Full wwPDB EM Validation Report

Oct 14, 2021 – 11:07 pm BST

PDB ID	:	7O1A
EMDB ID	:	EMD-12694
Title	:	Cryo-EM structure of an Escherichia coli TnaC(R23F)-ribosome complex stalled in response to L-tryptophan
Authors	:	van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.; Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera, L.R.; Innis, C.A.
Deposited on	:	2021-03-29
Resolution	:	2.40 Å(reported)
Based on initial model	:	6TBV

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

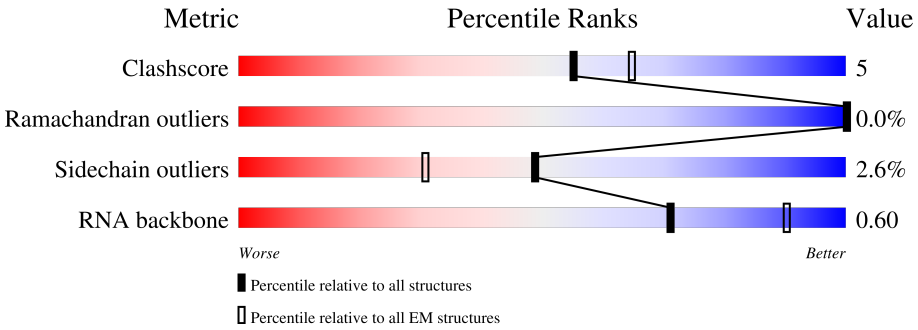
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AA	1534	55% 32% 12%
2	AB	240	10% 58% 32% 7%
3	AC	233	61% 25% 12%
4	AD	206	74% 23%
5	AE	167	73% 19% 7%
6	AF	135	59% 19% 21%
7	AG	179	57% 25% 16%

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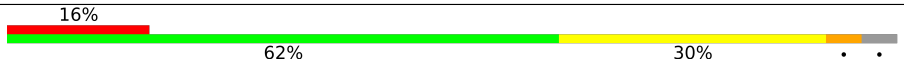
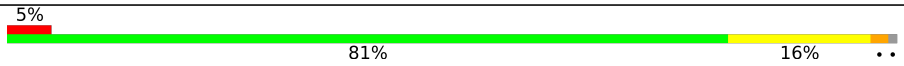
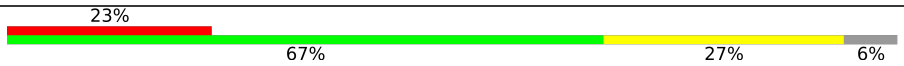
Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2897	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	
28	BG	177	
29	BH	149	
30	BI	70	
31	BJ	142	
32	BK	123	

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Mol	Chain	Length	Quality of chain
33	BL	144	88% 11%
34	BM	136	79% 19%
35	BN	127	80% 13% 7%
36	BO	117	87% 12%
37	BP	115	87% 11%
38	BQ	118	93% 6%
39	BR	103	91% 9%
40	BS	110	91% 9%
41	BT	100	74% 18% 7%
42	BU	104	83% 15%
43	BV	94	77% 23%
44	BW	85	74% 14% 11%
45	BX	78	87% 10%
46	BY	63	87% 10%
47	BZ	59	90% 8%
48	B0	57	77% 21%
49	B1	55	58% 35% 7%
50	B2	46	83% 17%
51	B3	65	86% 12%
52	B4	38	82% 18%
53	B5	17	76% 18% 6%
54	B7	9	56% 11% 33%
55	B8	77	42% 35% 19%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 146602 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called Ribosomal RNA 16S.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a protein called TnaC - Tryptophanase leader peptide - R23F.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B5	17	Total	C	N	O	0	0
			146	97	24	25		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B7	9	Total	C	N	O	P	0	0
			191	85	34	63	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B8	77	Total	C	N	O	P	0	0
			1648	735	295	541	77		

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

Mol	Chain	Residues	Atoms		AltConf
56	AA	86	Total	Mg	0
			86	86	
56	BA	233	Total	Mg	0
			233	233	
56	BB	1	Total	Mg	0
			1	1	
56	BC	1	Total	Mg	0
			1	1	
56	BD	2	Total	Mg	0
			2	2	
56	BL	1	Total	Mg	0
			1	1	
56	B8	2	Total	Mg	0
			2	2	

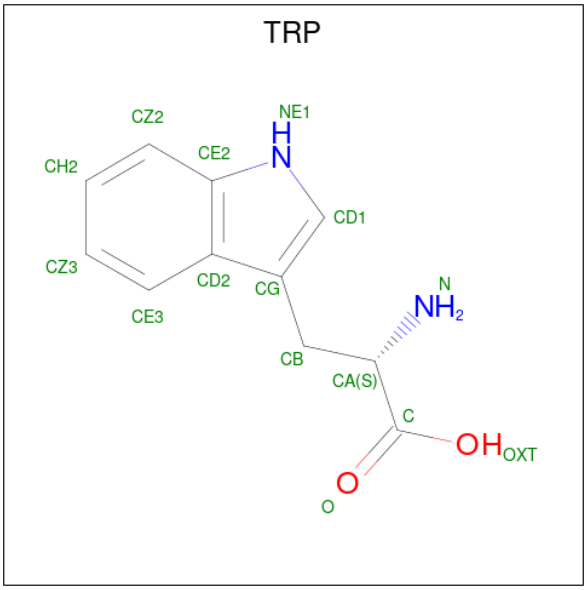
- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	AA	38	Total	K	0
			38	38	
57	AM	1	Total	K	0
			1	1	
57	BA	104	Total	K	0
			104	104	
57	BB	1	Total	K	0
			1	1	
57	BC	1	Total	K	0
			1	1	
57	BD	1	Total	K	0
			1	1	
57	BM	1	Total	K	0
			1	1	

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 59 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	AA	184	Total O 184 184	0
60	AK	1	Total O 1 1	0
60	AN	1	Total O 1 1	0
60	BA	1672	Total O 1672 1672	0
60	BB	2	Total O 2 2	0
60	BC	38	Total O 38 38	0

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Mol	Chain	Residues	Atoms	AltConf
60	BD	14	Total O 14 14	0
60	BE	21	Total O 21 21	0
60	BF	1	Total O 1 1	0
60	BJ	2	Total O 2 2	0
60	BK	3	Total O 3 3	0
60	BL	14	Total O 14 14	0
60	BM	2	Total O 2 2	0
60	BN	9	Total O 9 9	0
60	BO	1	Total O 1 1	0
60	BP	2	Total O 2 2	0
60	BQ	12	Total O 12 12	0
60	BR	4	Total O 4 4	0
60	BS	7	Total O 7 7	0
60	BT	3	Total O 3 3	0
60	BU	1	Total O 1 1	0
60	BW	5	Total O 5 5	0
60	BX	4	Total O 4 4	0
60	B0	4	Total O 4 4	0
60	B2	6	Total O 6 6	0
60	B3	7	Total O 7 7	0
60	B4	1	Total O 1 1	0

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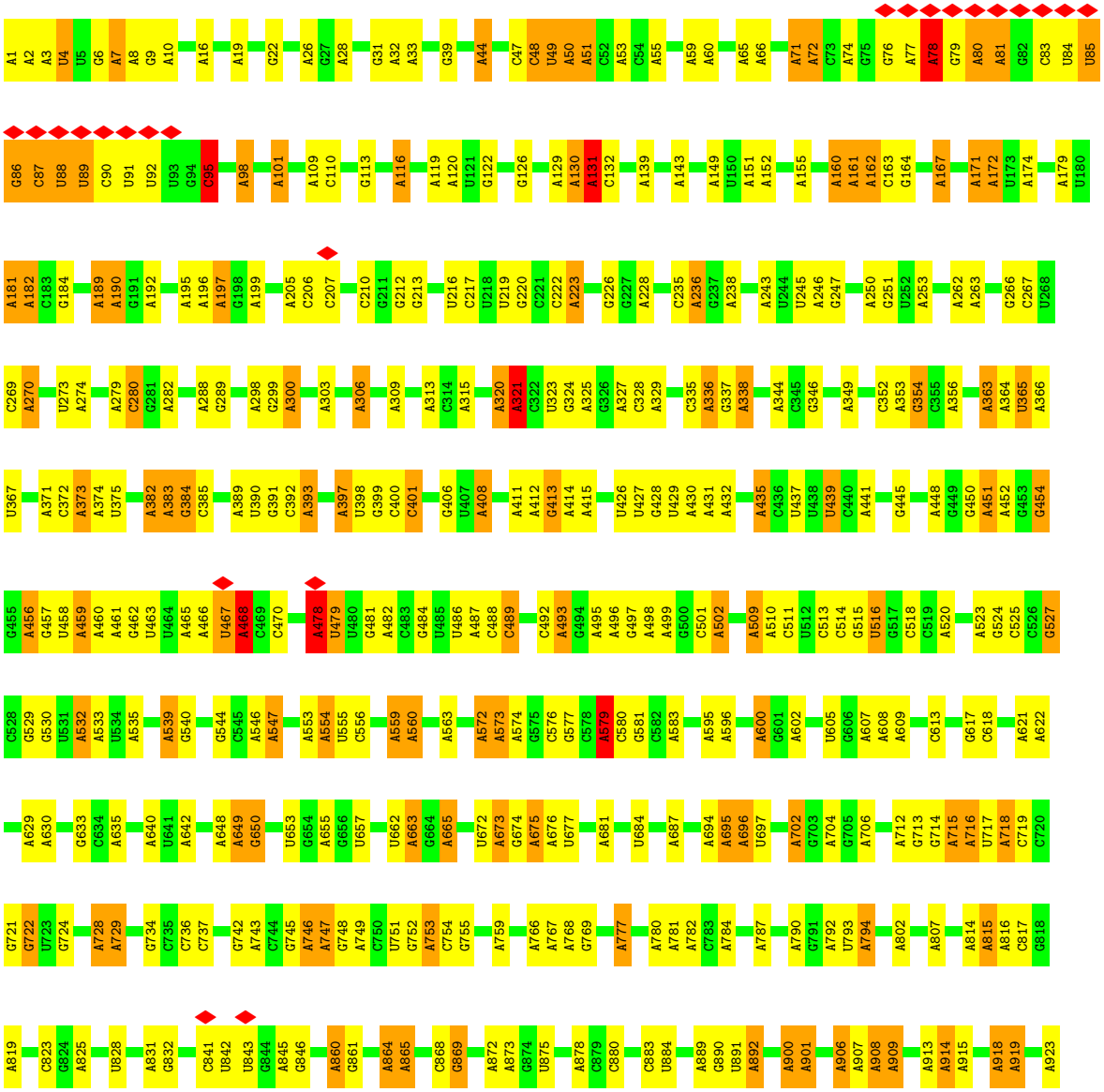
Mol	Chain	Residues	Atoms	AltConf
60	B5	2	Total O 2 2	0
60	B8	3	Total O 3 3	0

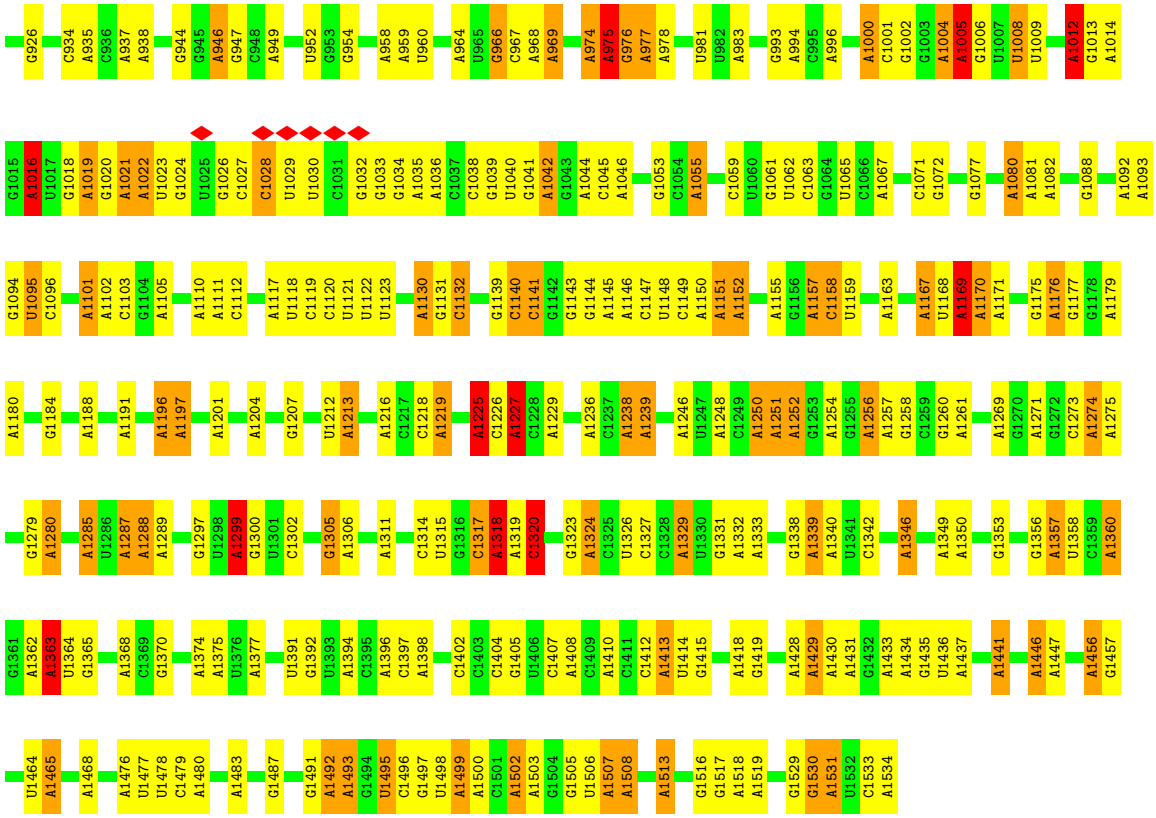
3 Residue-property plots (i)

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

- Molecule 1: Ribosomal RNA 16S

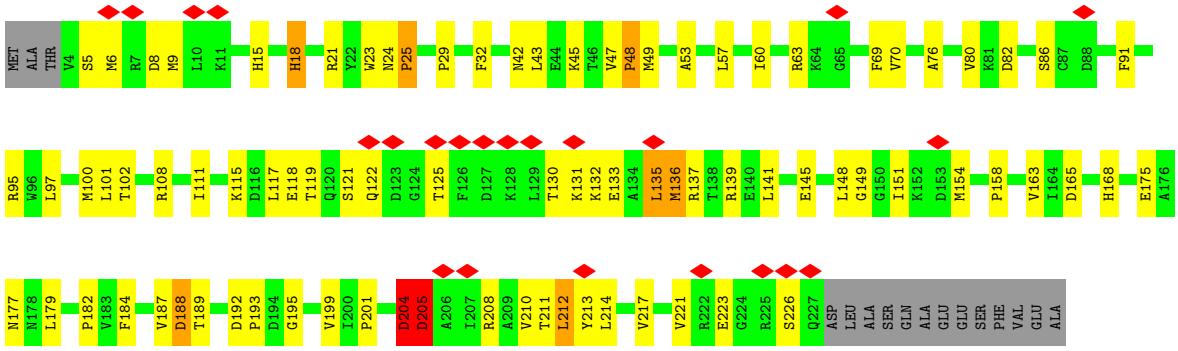
Chain AA:





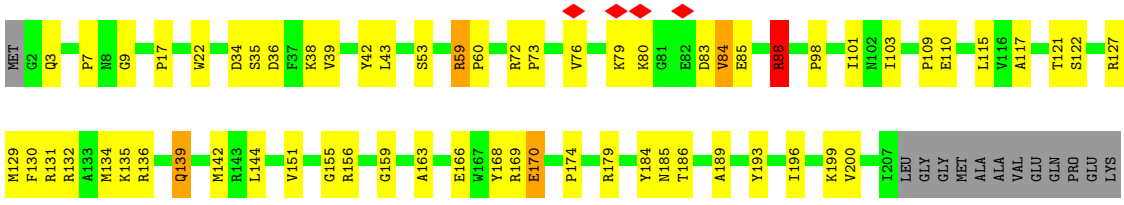
• Molecule 2: 30S ribosomal protein S2

Chain AB:



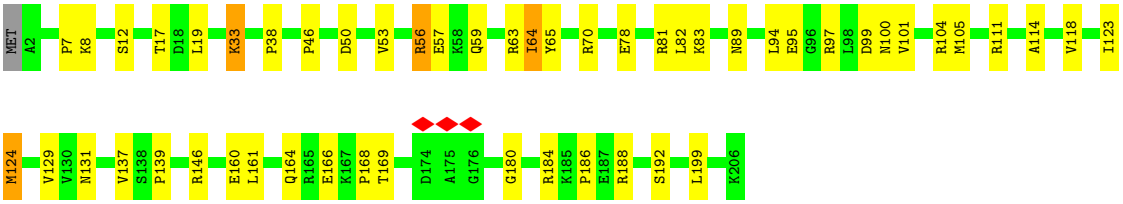
• Molecule 3: 30S ribosomal protein S3

Chain AC:



• Molecule 4: 30S ribosomal protein S4

Chain AD:

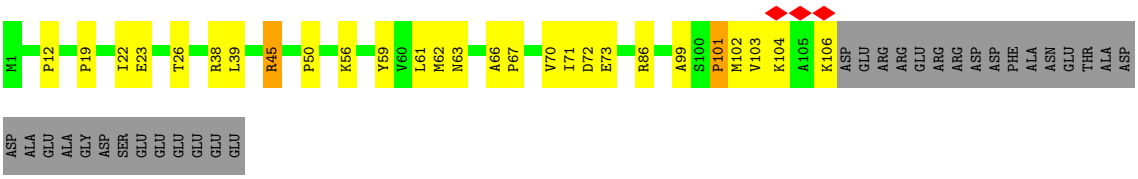


• Molecule 5: 30S ribosomal protein S5

Chain AE:

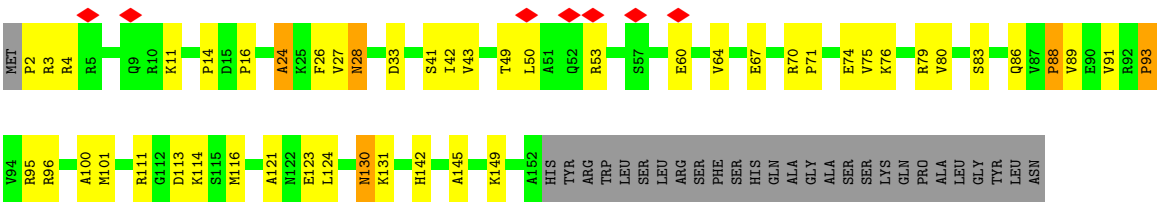
• Molecule 6: 30S ribosomal protein S6

Chain AF:



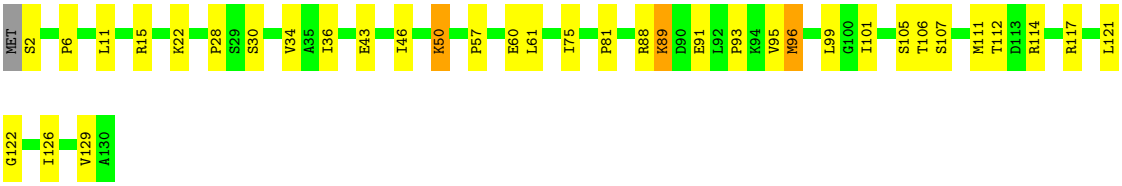
• Molecule 7: 30S ribosomal protein S7

Chain AG:

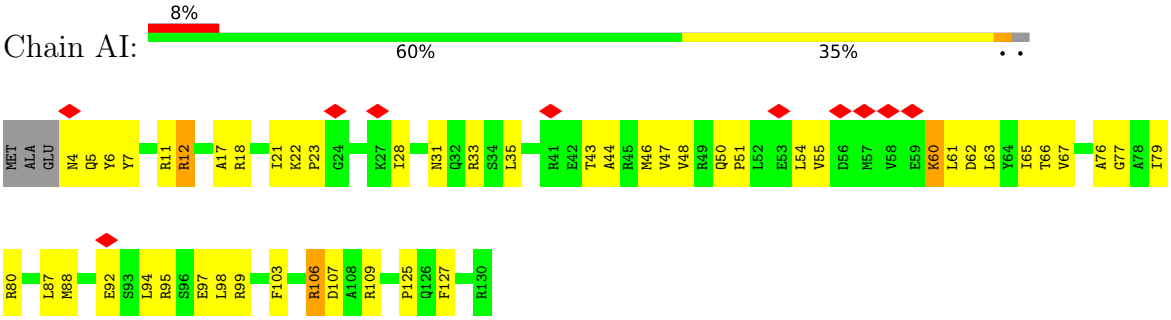


• Molecule 8: 30S ribosomal protein S8

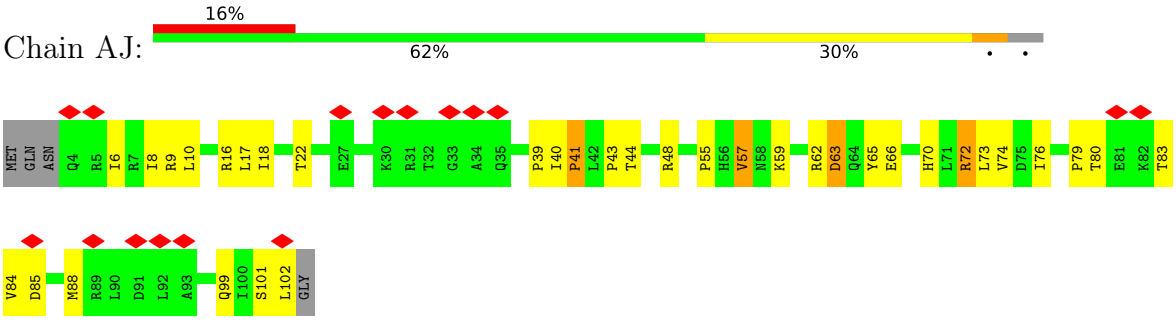
Chain AH:



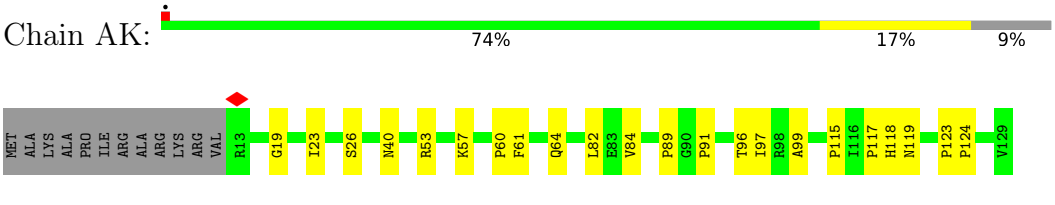
• Molecule 9: 30S ribosomal protein S9



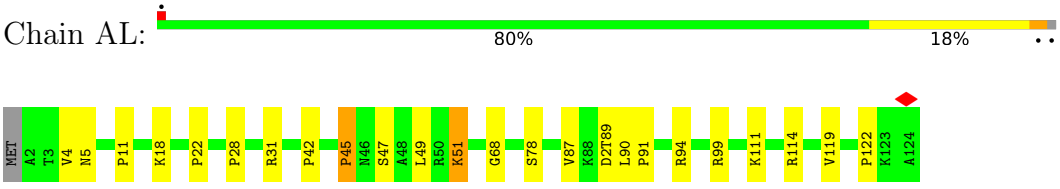
• Molecule 10: 30S ribosomal protein S10



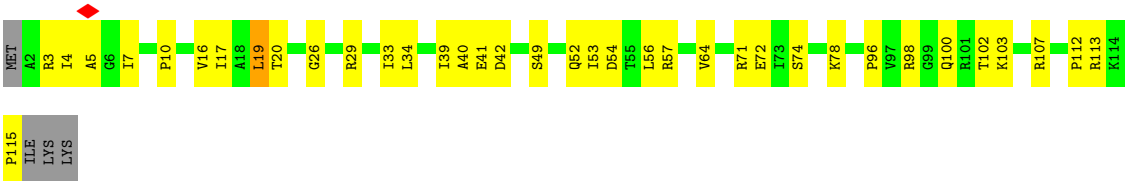
• Molecule 11: 30S ribosomal protein S11



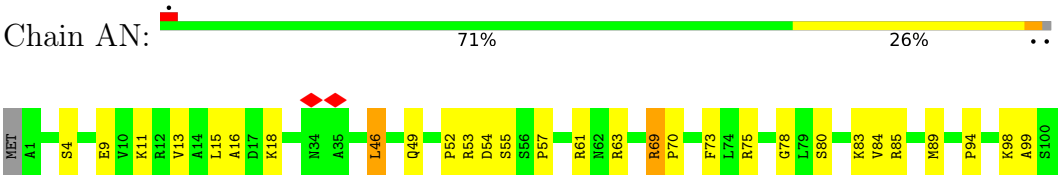
• Molecule 12: 30S ribosomal protein S12



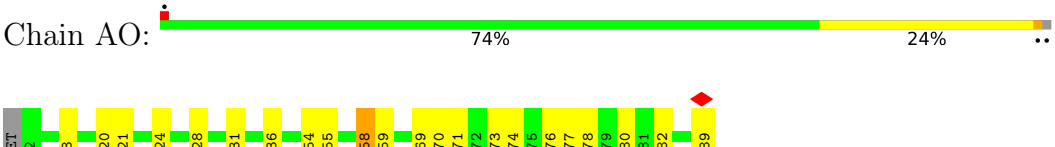
• Molecule 13: 30S ribosomal protein S13



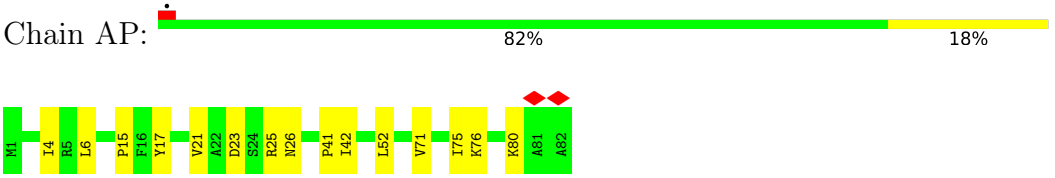
• Molecule 14: 30S ribosomal protein S14



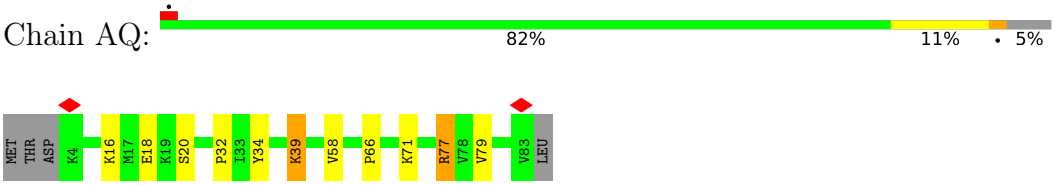
• Molecule 15: 30S ribosomal protein S15



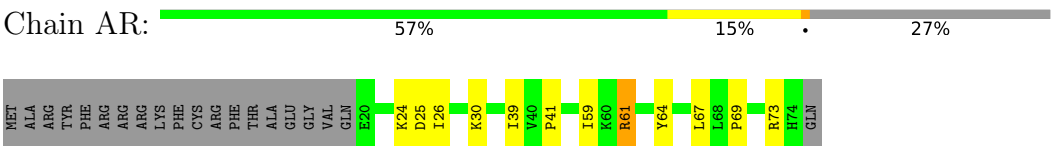
• Molecule 16: 30S ribosomal protein S16



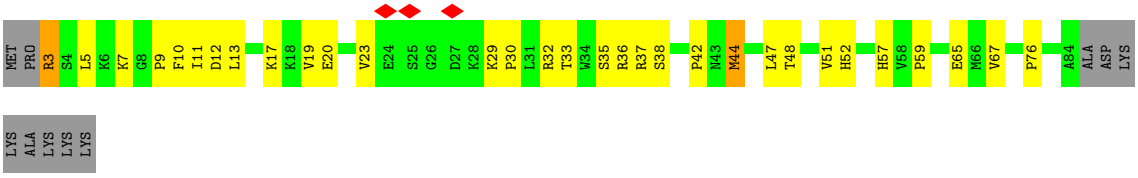
• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

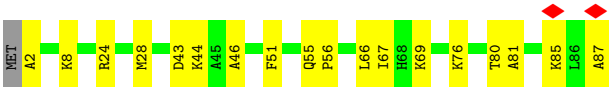


• Molecule 19: 30S ribosomal protein S19



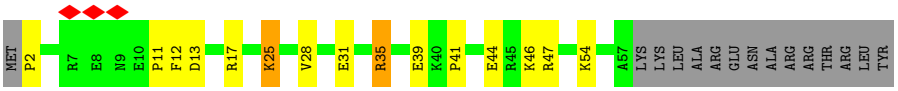
• Molecule 20: 30S ribosomal protein S20

Chain AT:



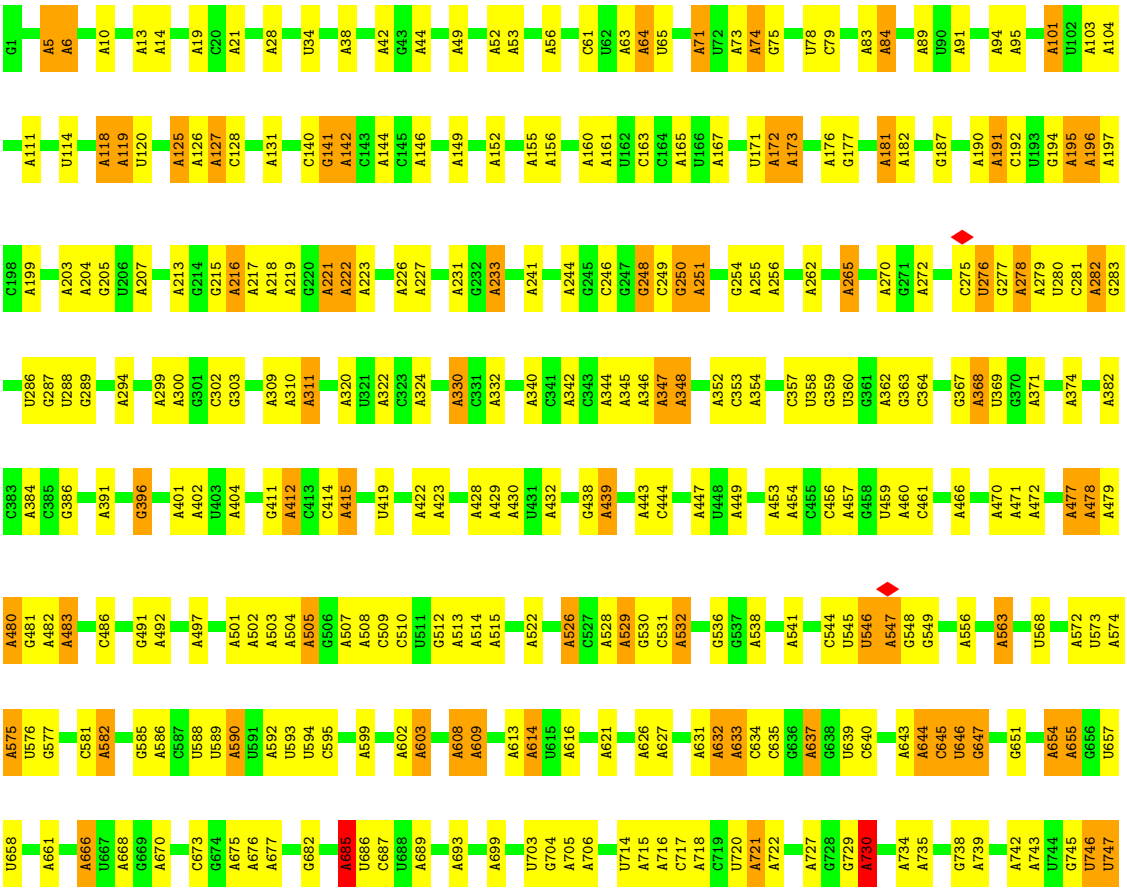
• Molecule 21: 30S ribosomal protein S21

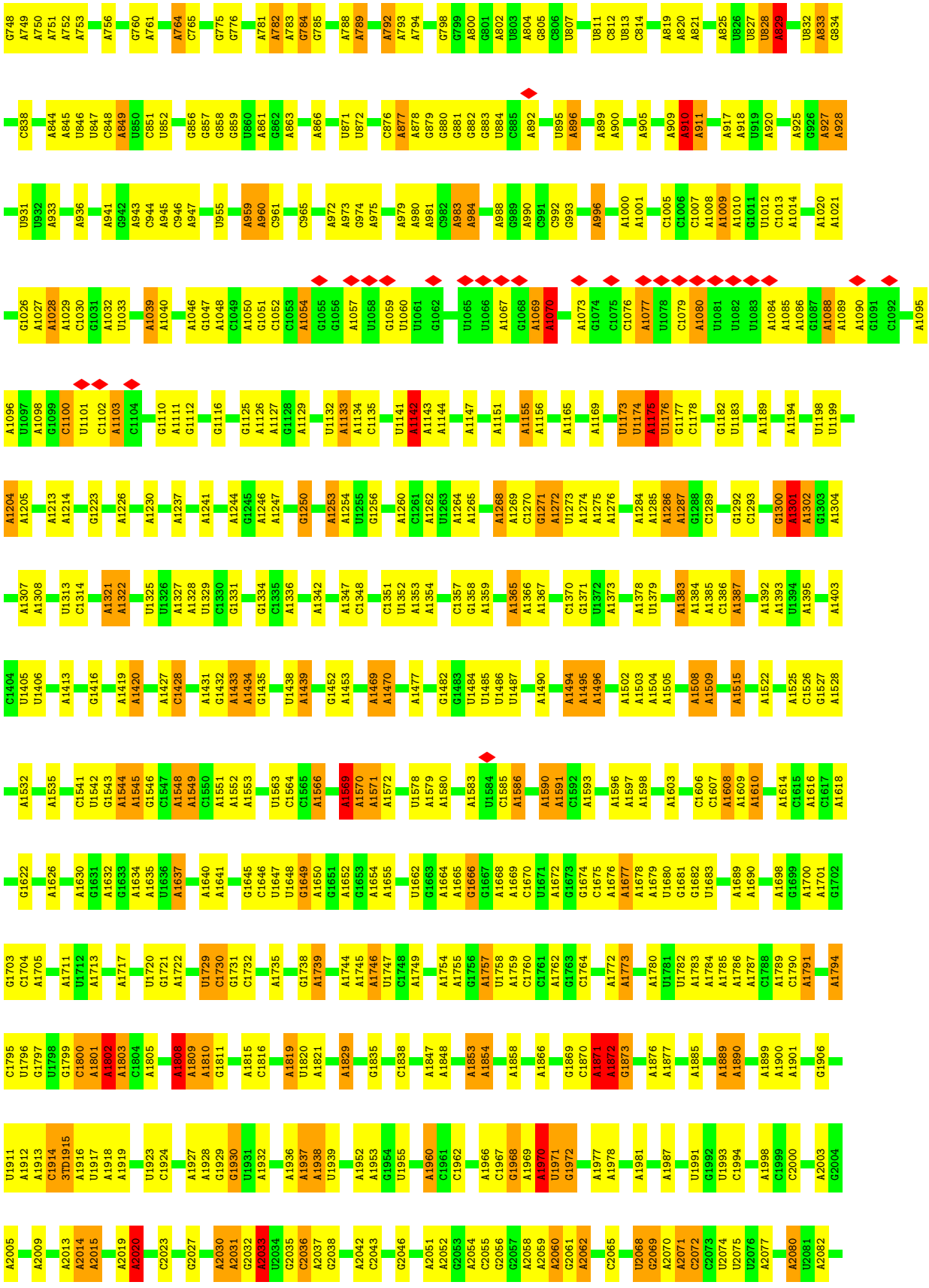
Chain AU:

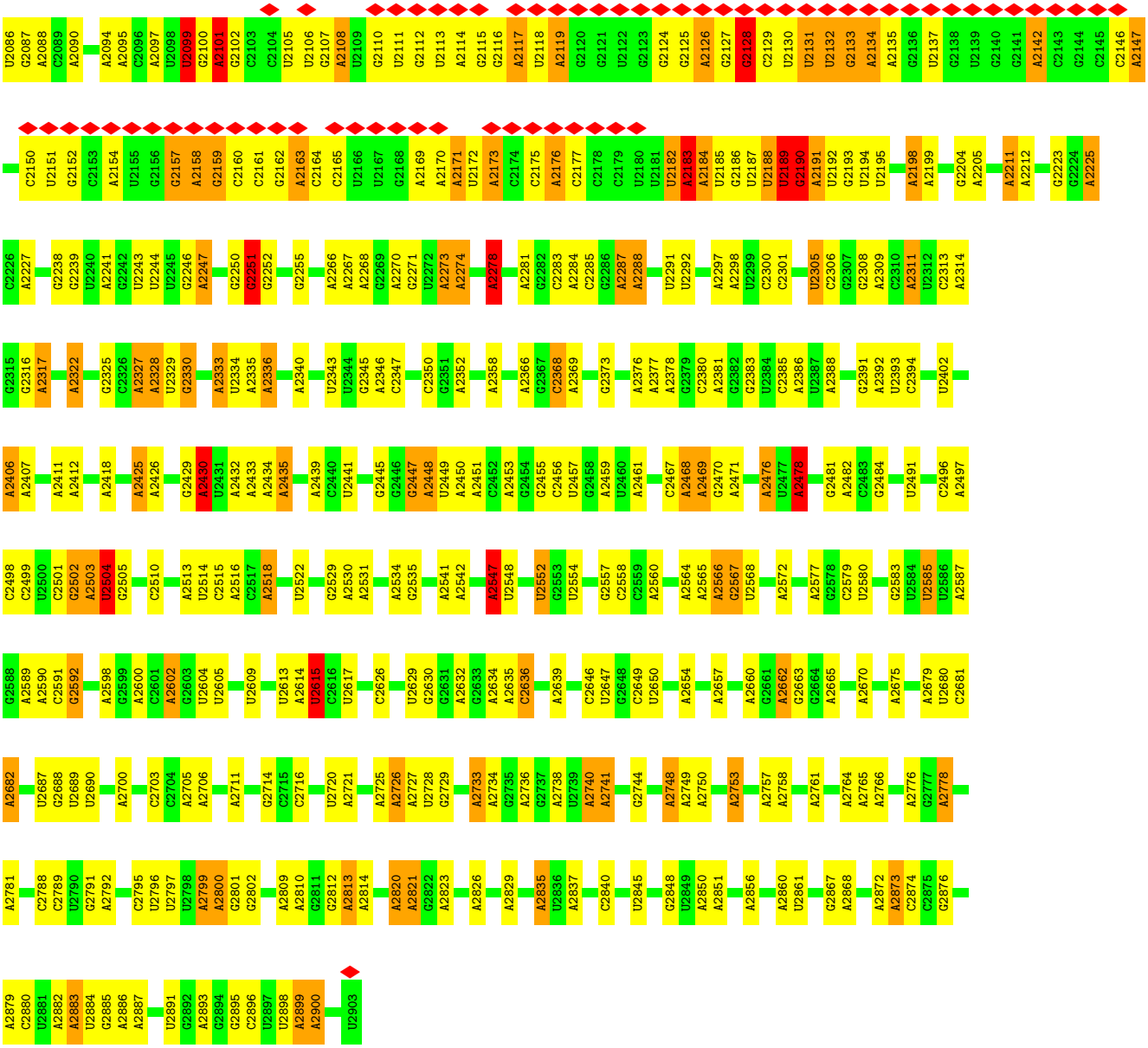


• Molecule 22: Ribosomal RNA 23S

Chain BA:

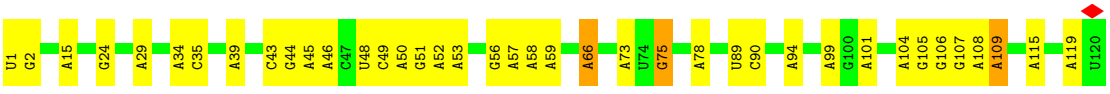






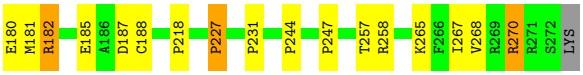
• Molecule 23: Ribosomal RNA 5S

Chain BB:

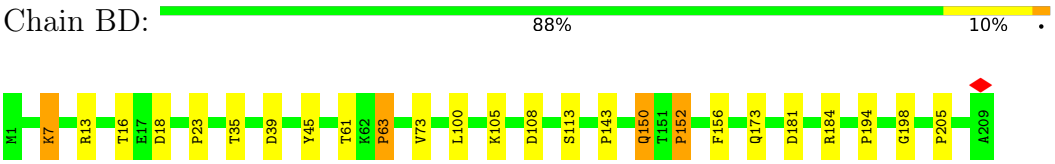


• Molecule 24: 50S ribosomal protein L2

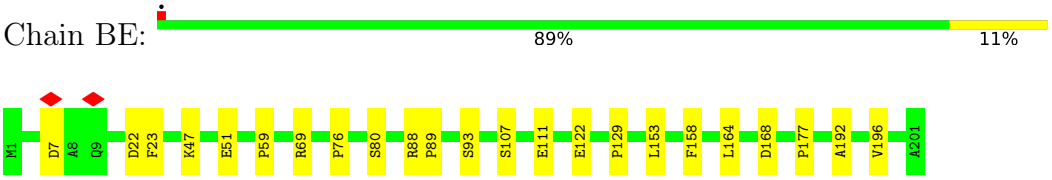
Chain BC:



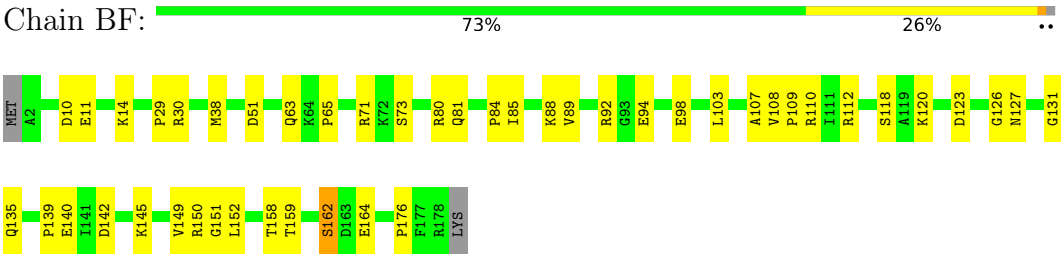
• Molecule 25: 50S ribosomal protein L3



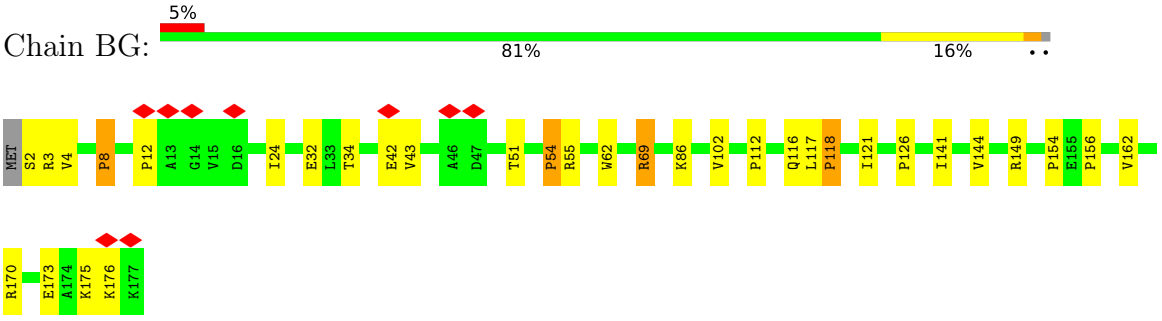
• Molecule 26: 50S ribosomal protein L4



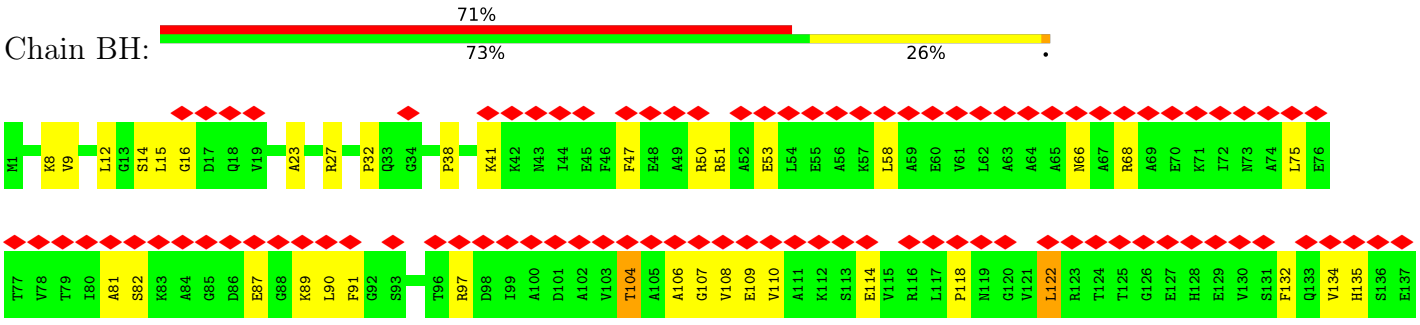
• Molecule 27: 50S ribosomal protein L5

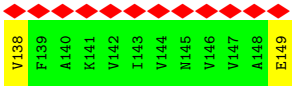


• Molecule 28: 50S ribosomal protein L6



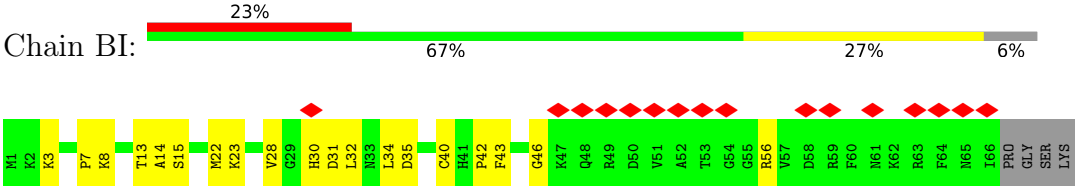
• Molecule 29: 50S ribosomal protein L9





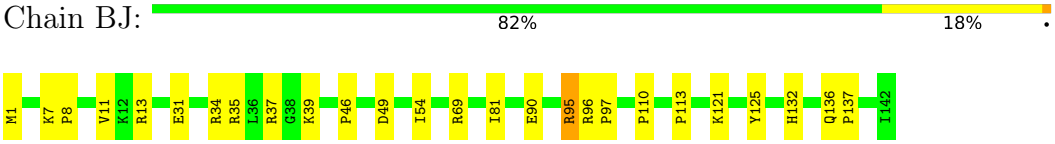
• Molecule 30: 50S ribosomal protein L31

Chain BI:



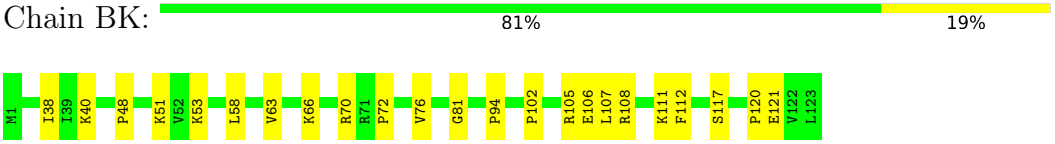
• Molecule 31: 50S ribosomal protein L13

Chain BJ:



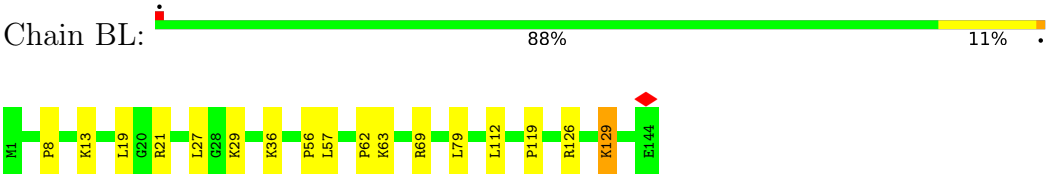
• Molecule 32: 50S ribosomal protein L14

Chain BK:



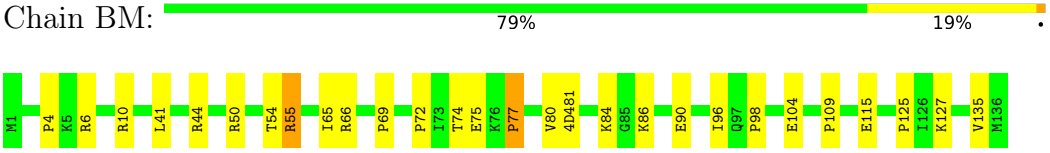
• Molecule 33: 50S ribosomal protein L15

Chain BL:



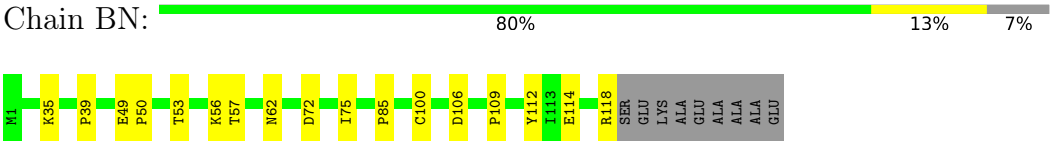
• Molecule 34: 50S ribosomal protein L16

Chain BM:



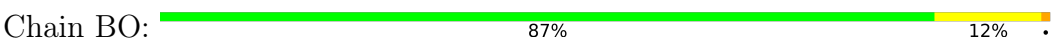
• Molecule 35: 50S ribosomal protein L17

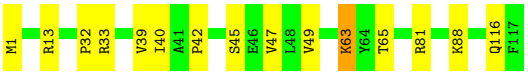
Chain BN:



• Molecule 36: 50S ribosomal protein L18

Chain BO:



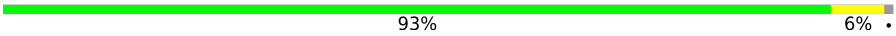


• Molecule 37: 50S ribosomal protein L19

Chain BP:

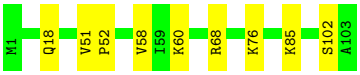
• Molecule 38: 50S ribosomal protein L20

Chain BQ:



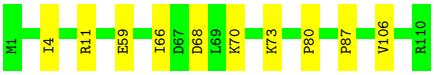
• Molecule 39: 50S ribosomal protein L21

Chain BR:



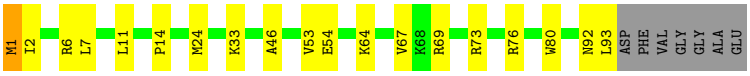
• Molecule 40: 50S ribosomal protein L22

Chain BS:



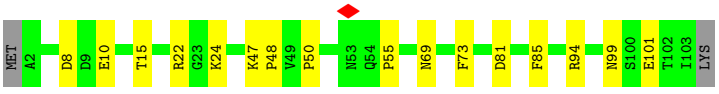
• Molecule 41: 50S ribosomal protein L23

Chain BT:



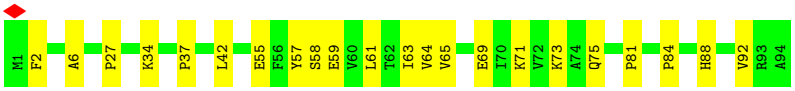
• Molecule 42: 50S ribosomal protein L24

Chain BU:

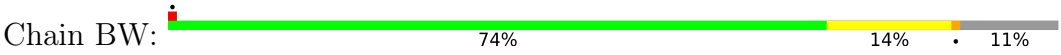


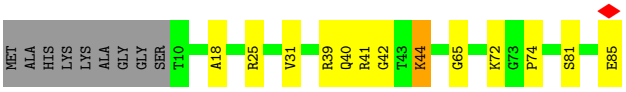
• Molecule 43: 50S ribosomal protein L25

Chain BV:

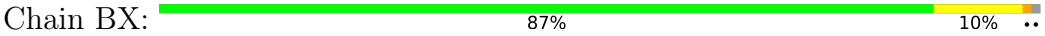


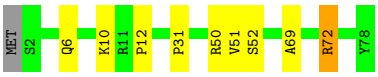
• Molecule 44: 50S ribosomal protein L27



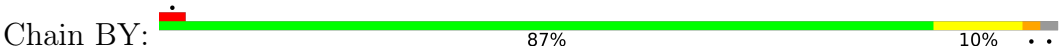


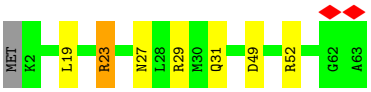
• Molecule 45: 50S ribosomal protein L28



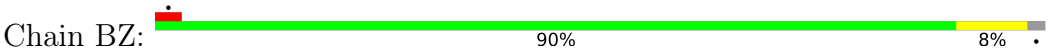


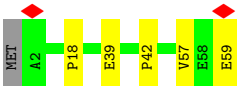
• Molecule 46: 50S ribosomal protein L29



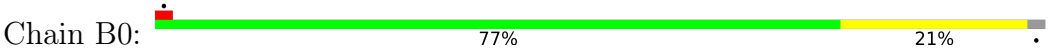


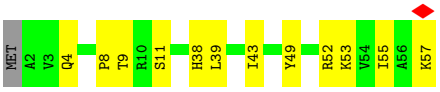
• Molecule 47: 50S ribosomal protein L30



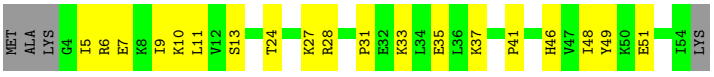


• Molecule 48: 50S ribosomal protein L32



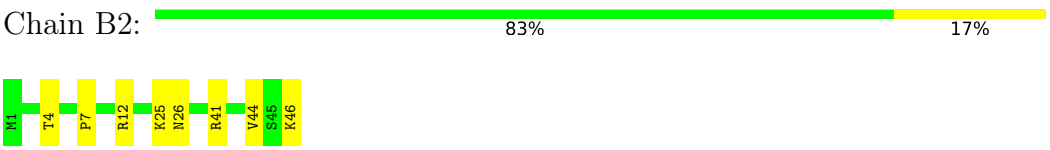


• Molecule 49: 50S ribosomal protein L33



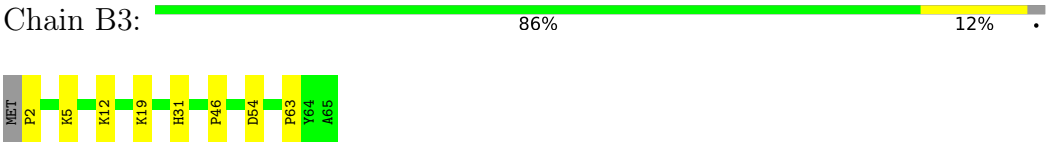
• Molecule 50: 50S ribosomal protein L34

Chain B2:



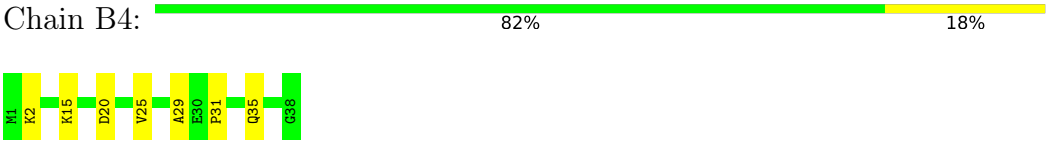
• Molecule 51: 50S ribosomal protein L35

Chain B3:



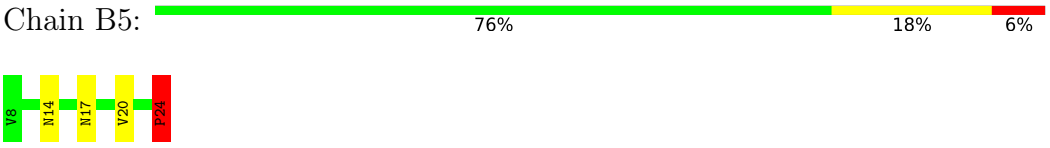
• Molecule 52: 50S ribosomal protein L36

Chain B4:



• Molecule 53: TnaC - Tryptophanase leader peptide - R23F

Chain B5:

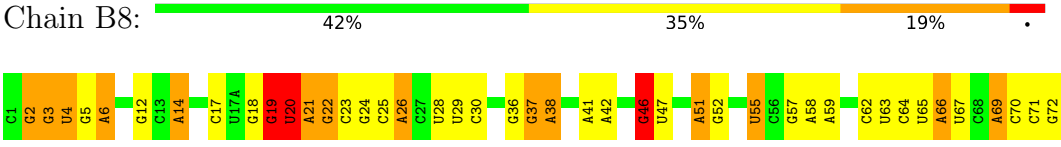


• Molecule 54: mRNA

Chain B7:

• Molecule 55: P-site tRNA-Pro

Chain B8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	191230	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-1600	Depositor
Magnification	59880	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0075	Depositor
Map size (Å)	271.375, 271.375, 271.375	wwPDB
Map dimensions	325, 325, 325	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	1.48	1296/36593 (3.5%)	3.33	3996/57081 (7.0%)
2	AB	0.90	9/1784 (0.5%)	1.10	13/2403 (0.5%)
3	AC	0.86	7/1651 (0.4%)	0.69	3/2225 (0.1%)
4	AD	0.80	6/1665 (0.4%)	0.65	2/2227 (0.1%)
5	AE	0.87	5/1157 (0.4%)	0.61	1/1557 (0.1%)
6	AF	0.94	5/881 (0.6%)	0.58	0/1189
7	AG	0.99	8/1195 (0.7%)	0.70	1/1602 (0.1%)
8	AH	0.96	6/989 (0.6%)	0.69	2/1326 (0.2%)
9	AI	0.73	3/1034 (0.3%)	0.72	2/1375 (0.1%)
10	AJ	1.08	6/805 (0.7%)	0.74	0/1089
11	AK	1.12	7/893 (0.8%)	0.67	0/1205
12	AL	1.09	8/960 (0.8%)	0.62	0/1286
13	AM	0.91	5/892 (0.6%)	0.74	2/1193 (0.2%)
14	AN	0.90	4/811 (0.5%)	0.63	1/1081 (0.1%)
15	AO	0.32	0/722	0.53	0/964
16	AP	0.73	2/659 (0.3%)	0.57	0/884
17	AQ	0.73	2/657 (0.3%)	0.77	2/881 (0.2%)
18	AR	0.84	2/462 (0.4%)	0.58	0/621
19	AS	1.08	5/672 (0.7%)	0.78	2/904 (0.2%)
20	AT	0.56	1/676 (0.1%)	0.47	0/895
21	AU	1.15	5/472 (1.1%)	0.62	0/627
22	BA	1.57	2305/69121 (3.3%)	3.43	7802/107828 (7.2%)
23	BB	1.34	75/2872 (2.6%)	2.95	243/4478 (5.4%)
24	BC	1.14	17/2121 (0.8%)	0.65	0/2852
25	BD	0.86	8/1576 (0.5%)	0.56	0/2119
26	BE	0.76	5/1571 (0.3%)	0.55	0/2113
27	BF	0.84	6/1434 (0.4%)	0.63	2/1926 (0.1%)
28	BG	0.98	8/1343 (0.6%)	0.59	0/1816
29	BH	0.71	3/1121 (0.3%)	0.67	2/1515 (0.1%)
30	BI	0.82	2/531 (0.4%)	0.70	1/709 (0.1%)
31	BJ	0.92	6/1152 (0.5%)	0.55	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BK	0.93	5/955 (0.5%)	0.63	0/1279
33	BL	0.83	4/1062 (0.4%)	0.58	0/1413
34	BM	1.02	7/1081 (0.6%)	0.59	0/1443
35	BN	0.86	4/958 (0.4%)	0.61	0/1281
36	BO	0.65	2/910 (0.2%)	0.50	0/1219
37	BP	0.80	3/929 (0.3%)	0.56	0/1242
38	BQ	0.38	0/960	0.50	0/1278
39	BR	0.63	2/829 (0.2%)	0.56	0/1107
40	BS	0.69	2/864 (0.2%)	0.59	0/1156
41	BT	0.64	1/744 (0.1%)	0.78	4/994 (0.4%)
42	BU	0.82	3/787 (0.4%)	0.58	0/1051
43	BV	0.92	4/766 (0.5%)	0.56	0/1025
44	BW	0.64	1/587 (0.2%)	0.55	0/776
45	BX	0.77	2/635 (0.3%)	0.55	0/848
46	BY	0.30	0/502	0.45	0/667
47	BZ	0.84	2/453 (0.4%)	0.54	0/605
48	B0	0.65	1/450 (0.2%)	0.58	0/599
49	B1	0.92	2/421 (0.5%)	0.60	0/561
50	B2	0.75	1/380 (0.3%)	0.56	0/498
51	B3	1.13	4/513 (0.8%)	0.61	0/676
52	B4	0.79	1/303 (0.3%)	0.55	0/397
53	B5	1.33	2/151 (1.3%)	0.90	1/205 (0.5%)
54	B7	1.51	6/212 (2.8%)	2.52	12/328 (3.7%)
55	B8	1.53	41/1765 (2.3%)	3.06	169/2750 (6.1%)
All	All	1.38	3927/155689 (2.5%)	2.93	12263/232920 (5.3%)

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	AB	0	2
7	AG	0	1
29	BH	0	2
43	BV	0	1
All	All	0	6

All (3927) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2449	U	C5-C6	23.39	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	B8	20	U	C5-C6	22.49	1.54	1.34
10	AJ	41	PRO	N-CD	12.96	1.66	1.47
7	AG	2	PRO	N-CD	12.92	1.66	1.47
21	AU	2	PRO	N-CD	12.52	1.65	1.47
51	B3	63	PRO	N-CD	12.17	1.64	1.47
12	AL	45	PRO	N-CD	12.15	1.64	1.47
24	BC	11	PRO	N-CD	12.09	1.64	1.47
10	AJ	39	PRO	N-CD	12.08	1.64	1.47
29	BH	118	PRO	N-CD	12.04	1.64	1.47
25	BD	152	PRO	N-CD	12.02	1.64	1.47
39	BR	52	PRO	N-CD	12.01	1.64	1.47
28	BG	156	PRO	N-CD	11.95	1.64	1.47
24	BC	8	PRO	N-CD	11.93	1.64	1.47
11	AK	117	PRO	N-CD	11.89	1.64	1.47
3	AC	174	PRO	N-CD	11.83	1.64	1.47
8	AH	93	PRO	N-CD	11.80	1.64	1.47
2	AB	29	PRO	N-CD	11.80	1.64	1.47
27	BF	84	PRO	N-CD	11.79	1.64	1.47
7	AG	14	PRO	N-CD	11.78	1.64	1.47
51	B3	2	PRO	N-CD	11.77	1.64	1.47
13	AM	115	PRO	N-CD	11.76	1.64	1.47
33	BL	8	PRO	N-CD	11.75	1.64	1.47
5	AE	150	PRO	N-CD	11.74	1.64	1.47
21	AU	11	PRO	N-CD	11.72	1.64	1.47
8	AH	6	PRO	N-CD	11.72	1.64	1.47
10	AJ	79	PRO	N-CD	11.72	1.64	1.47
50	B2	7	PRO	N-CD	11.67	1.64	1.47
40	BS	87	PRO	N-CD	11.61	1.64	1.47
25	BD	23	PRO	N-CD	11.60	1.64	1.47
35	BN	85	PRO	N-CD	11.60	1.64	1.47
5	AE	98	PRO	N-CD	11.59	1.64	1.47
36	BO	32	PRO	N-CD	11.56	1.64	1.47
20	AT	56	PRO	N-CD	11.56	1.64	1.47
3	AC	17	PRO	N-CD	11.55	1.64	1.47
2	AB	48	PRO	N-CD	11.55	1.64	1.47
7	AG	71	PRO	N-CD	11.54	1.64	1.47
4	AD	38	PRO	N-CD	11.53	1.64	1.47
43	BV	84	PRO	N-CD	11.51	1.64	1.47
24	BC	29	PRO	N-CD	11.50	1.64	1.47
53	B5	24	PRO	N-CD	11.49	1.64	1.47
14	AN	52	PRO	N-CD	11.49	1.64	1.47
34	BM	69	PRO	N-CD	11.49	1.64	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	BU	48	PRO	N-CD	11.48	1.64	1.47
28	BG	118	PRO	N-CD	11.45	1.63	1.47
2	AB	193	PRO	N-CD	11.45	1.63	1.47
28	BG	154	PRO	N-CD	11.45	1.63	1.47
24	BC	247	PRO	N-CD	11.44	1.63	1.47
41	BT	14	PRO	N-CD	11.42	1.63	1.47
14	AN	57	PRO	N-CD	11.41	1.63	1.47
11	AK	89	PRO	N-CD	11.39	1.63	1.47
42	BU	55	PRO	N-CD	11.39	1.63	1.47
44	BW	74	PRO	N-CD	11.38	1.63	1.47
49	B1	31	PRO	N-CD	11.38	1.63	1.47
3	AC	109	PRO	N-CD	11.38	1.63	1.47
6	AF	67	PRO	N-CD	11.33	1.63	1.47
24	BC	85	PRO	N-CD	11.32	1.63	1.47
18	AR	69	PRO	N-CD	11.32	1.63	1.47
24	BC	126	PRO	N-CD	11.32	1.63	1.47
2	AB	158	PRO	N-CD	11.31	1.63	1.47
7	AG	88	PRO	N-CD	11.31	1.63	1.47
4	AD	7	PRO	N-CD	11.30	1.63	1.47
28	BG	54	PRO	N-CD	11.28	1.63	1.47
31	BJ	137	PRO	N-CD	11.27	1.63	1.47
26	BE	129	PRO	N-CD	11.26	1.63	1.47
37	BP	18	PRO	N-CD	11.25	1.63	1.47
4	AD	186	PRO	N-CD	11.24	1.63	1.47
19	AS	42	PRO	N-CD	11.23	1.63	1.47
27	BF	29	PRO	N-CD	11.22	1.63	1.47
45	BX	12	PRO	N-CD	11.21	1.63	1.47
32	BK	102	PRO	N-CD	11.20	1.63	1.47
4	AD	46	PRO	N-CD	11.20	1.63	1.47
37	BP	22	PRO	N-CD	11.19	1.63	1.47
11	AK	91	PRO	N-CD	11.19	1.63	1.47
3	AC	7	PRO	N-CD	11.16	1.63	1.47
12	AL	22	PRO	N-CD	11.16	1.63	1.47
8	AH	28	PRO	N-CD	11.15	1.63	1.47
13	AM	96	PRO	N-CD	11.15	1.63	1.47
9	AI	23	PRO	N-CD	11.14	1.63	1.47
31	BJ	97	PRO	N-CD	11.14	1.63	1.47
51	B3	46	PRO	N-CD	11.13	1.63	1.47
34	BM	72	PRO	N-CD	11.12	1.63	1.47
34	BM	125	PRO	N-CD	11.11	1.63	1.47
27	BF	176	PRO	N-CD	11.10	1.63	1.47
33	BL	62	PRO	N-CD	11.10	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	BV	37	PRO	N-CD	11.09	1.63	1.47
2	AB	201	PRO	N-CD	11.09	1.63	1.47
11	AK	115	PRO	N-CD	11.08	1.63	1.47
11	AK	123	PRO	N-CD	11.07	1.63	1.47
24	BC	75	PRO	N-CD	11.06	1.63	1.47
43	BV	27	PRO	N-CD	11.06	1.63	1.47
10	AJ	43	PRO	N-CD	11.04	1.63	1.47
14	AN	70	PRO	N-CD	11.04	1.63	1.47
16	AP	41	PRO	N-CD	11.04	1.63	1.47
24	BC	32	PRO	N-CD	11.04	1.63	1.47
28	BG	126	PRO	N-CD	11.02	1.63	1.47
24	BC	107	PRO	N-CD	11.01	1.63	1.47
33	BL	119	PRO	N-CD	11.00	1.63	1.47
7	AG	93	PRO	N-CD	11.00	1.63	1.47
19	AS	59	PRO	N-CD	11.00	1.63	1.47
24	BC	22	PRO	N-CD	10.99	1.63	1.47
25	BD	194	PRO	N-CD	10.99	1.63	1.47
37	BP	79	PRO	N-CD	10.99	1.63	1.47
25	BD	63	PRO	N-CD	10.97	1.63	1.47
5	AE	57	PRO	N-CD	10.97	1.63	1.47
16	AP	15	PRO	N-CD	10.95	1.63	1.47
29	BH	32	PRO	N-CD	10.94	1.63	1.47
5	AE	84	PRO	N-CD	10.93	1.63	1.47
26	BE	89	PRO	N-CD	10.91	1.63	1.47
19	AS	30	PRO	N-CD	10.91	1.63	1.47
3	AC	60	PRO	N-CD	10.90	1.63	1.47
25	BD	205	PRO	N-CD	10.89	1.63	1.47
28	BG	112	PRO	N-CD	10.89	1.63	1.47
42	BU	50	PRO	N-CD	10.89	1.63	1.47
45	BX	31	PRO	N-CD	10.89	1.63	1.47
12	AL	42	PRO	N-CD	10.89	1.63	1.47
17	AQ	66	PRO	N-CD	10.89	1.63	1.47
13	AM	112	PRO	N-CD	10.88	1.63	1.47
2	AB	182	PRO	N-CD	10.87	1.63	1.47
8	AH	81	PRO	N-CD	10.88	1.63	1.47
12	AL	91	PRO	N-CD	10.88	1.63	1.47
30	BI	7	PRO	N-CD	10.85	1.63	1.47
26	BE	177	PRO	N-CD	10.84	1.63	1.47
12	AL	28	PRO	N-CD	10.84	1.63	1.47
33	BL	56	PRO	N-CD	10.83	1.63	1.47
36	BO	42	PRO	N-CD	10.82	1.63	1.47
26	BE	76	PRO	N-CD	10.81	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BM	4	PRO	N-CD	10.80	1.62	1.47
49	B1	41	PRO	N-CD	10.80	1.62	1.47
47	BZ	42	PRO	N-CD	10.80	1.62	1.47
2	AB	25	PRO	N-CD	10.79	1.62	1.47
26	BE	59	PRO	N-CD	10.79	1.62	1.47
19	AS	9	PRO	N-CD	10.79	1.62	1.47
19	AS	76	PRO	N-CD	10.79	1.62	1.47
6	AF	101	PRO	N-CD	10.78	1.62	1.47
3	AC	98	PRO	N-CD	10.77	1.62	1.47
4	AD	168	PRO	N-CD	10.75	1.62	1.47
21	AU	41	PRO	N-CD	10.75	1.62	1.47
35	BN	39	PRO	N-CD	10.75	1.62	1.47
24	BC	131	PRO	N-CD	10.75	1.62	1.47
25	BD	143	PRO	N-CD	10.74	1.62	1.47
11	AK	124	PRO	N-CD	10.72	1.62	1.47
31	BJ	113	PRO	N-CD	10.71	1.62	1.47
12	AL	122	PRO	N-CD	10.70	1.62	1.47
30	BI	42	PRO	N-CD	10.70	1.62	1.47
43	BV	81	PRO	N-CD	10.69	1.62	1.47
34	BM	109	PRO	N-CD	10.68	1.62	1.47
32	BK	120	PRO	N-CD	10.67	1.62	1.47
27	BF	139	PRO	N-CD	10.66	1.62	1.47
35	BN	109	PRO	N-CD	10.66	1.62	1.47
52	B4	31	PRO	N-CD	10.66	1.62	1.47
6	AF	50	PRO	N-CD	10.64	1.62	1.47
11	AK	60	PRO	N-CD	10.64	1.62	1.47
28	BG	12	PRO	N-CD	10.62	1.62	1.47
24	BC	148	PRO	N-CD	10.62	1.62	1.47
34	BM	77	PRO	N-CD	10.61	1.62	1.47
29	BH	38	PRO	N-CD	10.60	1.62	1.47
4	AD	139	PRO	N-CD	10.60	1.62	1.47
6	AF	19	PRO	N-CD	10.57	1.62	1.47
6	AF	12	PRO	N-CD	10.56	1.62	1.47
9	AI	51	PRO	N-CD	10.56	1.62	1.47
24	BC	244	PRO	N-CD	10.54	1.62	1.47
8	AH	57	PRO	N-CD	10.54	1.62	1.47
32	BK	72	PRO	N-CD	10.52	1.62	1.47
35	BN	50	PRO	N-CD	10.51	1.62	1.47
31	BJ	110	PRO	N-CD	10.48	1.62	1.47
27	BF	109	PRO	N-CD	10.46	1.62	1.47
12	AL	11	PRO	N-CD	10.39	1.62	1.47
27	BF	65	PRO	N-CD	10.38	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	218	PRO	N-CD	10.38	1.62	1.47
48	B0	8	PRO	N-CD	10.37	1.62	1.47
32	BK	94	PRO	N-CD	10.36	1.62	1.47
40	BS	80	PRO	N-CD	10.35	1.62	1.47
18	AR	41	PRO	N-CD	10.35	1.62	1.47
34	BM	98	PRO	N-CD	10.34	1.62	1.47
17	AQ	32	PRO	N-CD	10.33	1.62	1.47
24	BC	136	PRO	N-CD	10.29	1.62	1.47
28	BG	8	PRO	N-CD	10.27	1.62	1.47
9	AI	125	PRO	N-CD	10.27	1.62	1.47
10	AJ	55	PRO	N-CD	10.27	1.62	1.47
14	AN	94	PRO	N-CD	10.23	1.62	1.47
47	BZ	18	PRO	N-CD	10.19	1.62	1.47
13	AM	10	PRO	N-CD	10.19	1.62	1.47
3	AC	73	PRO	N-CD	10.14	1.62	1.47
7	AG	16	PRO	N-CD	10.14	1.62	1.47
32	BK	48	PRO	N-CD	10.13	1.62	1.47
31	BJ	46	PRO	N-CD	10.12	1.62	1.47
22	BA	2449	U	N1-C6	10.08	1.47	1.38
55	B8	20	U	N1-C6	10.07	1.47	1.38
1	AA	412	A	C8-N7	10.03	1.38	1.31
24	BC	227	PRO	N-CD	9.99	1.61	1.47
5	AE	133	PRO	N-CD	9.95	1.61	1.47
31	BJ	8	PRO	N-CD	9.90	1.61	1.47
22	BA	2451	A	C8-N7	9.88	1.38	1.31
54	B7	7	U	O3'-P	-9.82	1.49	1.61
24	BC	231	PRO	N-CD	9.59	1.61	1.47
1	AA	622	A	C8-N7	9.33	1.38	1.31
1	AA	1446	A	C8-N7	9.28	1.38	1.31
1	AA	1004	A	C8-N7	9.26	1.38	1.31
1	AA	460	A	C8-N7	9.20	1.38	1.31
22	BA	1847	A	C8-N7	9.17	1.38	1.31
1	AA	431	A	C8-N7	9.02	1.37	1.31
55	B8	20	U	C4-C5	8.97	1.51	1.43
1	AA	74	A	C8-N7	8.86	1.37	1.31
22	BA	1848	A	C8-N7	8.86	1.37	1.31
1	AA	1332	A	C8-N7	8.84	1.37	1.31
1	AA	274	A	C8-N7	8.80	1.37	1.31
51	B3	2	PRO	N-CA	-8.78	1.32	1.47
1	AA	1213	A	C8-N7	8.78	1.37	1.31
7	AG	2	PRO	N-CA	-8.78	1.32	1.47
1	AA	253	A	C8-N7	8.77	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	461	A	C8-N7	8.73	1.37	1.31
2	AB	204	ASP	CB-CG	-8.66	1.33	1.51
1	AA	1340	A	C8-N7	8.57	1.37	1.31
1	AA	1204	A	C8-N7	8.51	1.37	1.31
22	BA	2872	A	C8-N7	8.51	1.37	1.31
22	BA	1739	A	C8-N7	8.49	1.37	1.31
22	BA	2101	A	C8-N7	8.49	1.37	1.31
22	BA	2117	A	C8-N7	8.45	1.37	1.31
22	BA	2449	U	C4-C5	8.43	1.51	1.43
1	AA	996	A	C8-N7	8.42	1.37	1.31
1	AA	1500	A	C8-N7	8.42	1.37	1.31
1	AA	1447	A	C8-N7	8.41	1.37	1.31
22	BA	821	A	C5-C4	-8.41	1.32	1.38
1	AA	152	A	C8-N7	8.39	1.37	1.31
21	AU	2	PRO	N-CA	-8.37	1.33	1.47
22	BA	1077	A	C8-N7	8.37	1.37	1.31
1	AA	958	A	C8-N7	8.34	1.37	1.31
1	AA	554	A	C8-N7	8.33	1.37	1.31
22	BA	1070	A	C8-N7	8.33	1.37	1.31
1	AA	1239	A	C8-N7	8.32	1.37	1.31
22	BA	2147	A	C8-N7	8.31	1.37	1.31
22	BA	2119	A	C8-N7	8.30	1.37	1.31
22	BA	1420	A	C8-N7	8.29	1.37	1.31
1	AA	459	A	C8-N7	8.29	1.37	1.31
22	BA	2430	A	C8-N7	8.29	1.37	1.31
22	BA	10	A	C8-N7	8.28	1.37	1.31
1	AA	1130	A	C8-N7	8.28	1.37	1.31
1	AA	1534	A	C8-N7	8.28	1.37	1.31
22	BA	2191	A	C8-N7	8.27	1.37	1.31
1	AA	1005	A	C8-N7	8.27	1.37	1.31
22	BA	354	A	C8-N7	8.27	1.37	1.31
22	BA	352	A	C8-N7	8.26	1.37	1.31
22	BA	959	A	C5-C4	-8.25	1.32	1.38
1	AA	408	A	C8-N7	8.24	1.37	1.31
22	BA	1080	A	C8-N7	8.24	1.37	1.31
1	AA	665	A	C8-N7	8.24	1.37	1.31
22	BA	1603	A	C5-C4	-8.24	1.32	1.38
1	AA	1329	A	C8-N7	8.23	1.37	1.31
22	BA	1583	A	C8-N7	8.23	1.37	1.31
1	AA	1044	A	C8-N7	8.22	1.37	1.31
22	BA	1089	A	C8-N7	8.22	1.37	1.31
1	AA	196	A	C8-N7	8.21	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1353	A	C5-C4	-8.19	1.33	1.38
22	BA	2171	A	C8-N7	8.19	1.37	1.31
1	AA	1346	A	C8-N7	8.19	1.37	1.31
1	AA	1257	A	C8-N7	8.18	1.37	1.31
1	AA	1179	A	C8-N7	8.18	1.37	1.31
22	BA	279	A	C8-N7	8.17	1.37	1.31
22	BA	1434	A	C8-N7	8.17	1.37	1.31
1	AA	182	A	C8-N7	8.17	1.37	1.31
1	AA	520	A	C8-N7	8.15	1.37	1.31
1	AA	1151	A	C8-N7	8.14	1.37	1.31
1	AA	81	A	C8-N7	8.13	1.37	1.31
1	AA	171	A	C8-N7	8.13	1.37	1.31
1	AA	1188	A	C8-N7	8.12	1.37	1.31
1	AA	1016	A	C8-N7	8.12	1.37	1.31
1	AA	1042	A	C8-N7	8.11	1.37	1.31
1	AA	1019	A	C8-N7	8.11	1.37	1.31
22	BA	1057	A	C8-N7	8.11	1.37	1.31
22	BA	1050	A	C8-N7	8.10	1.37	1.31
1	AA	192	A	C8-N7	8.09	1.37	1.31
1	AA	1377	A	C8-N7	8.08	1.37	1.31
22	BA	1046	A	C8-N7	8.08	1.37	1.31
1	AA	1360	A	C8-N7	8.08	1.37	1.31
22	BA	547	A	C8-N7	8.07	1.37	1.31
1	AA	371	A	C8-N7	8.06	1.37	1.31
1	AA	366	A	C8-N7	8.06	1.37	1.31
1	AA	189	A	C8-N7	8.06	1.37	1.31
1	AA	195	A	C8-N7	8.05	1.37	1.31
1	AA	1150	A	C8-N7	8.04	1.37	1.31
1	AA	452	A	C8-N7	8.04	1.37	1.31
1	AA	1287	A	C8-N7	8.04	1.37	1.31
1	AA	1288	A	C8-N7	8.04	1.37	1.31
23	BB	119	A	C8-N7	8.04	1.37	1.31
1	AA	1000	A	C8-N7	8.04	1.37	1.31
1	AA	1299	A	C8-N7	8.03	1.37	1.31
22	BA	2211	A	C8-N7	8.03	1.37	1.31
1	AA	389	A	C8-N7	8.03	1.37	1.31
1	AA	414	A	C8-N7	8.03	1.37	1.31
22	BA	877	A	C8-N7	8.03	1.37	1.31
54	B7	9	A	C8-N7	8.03	1.37	1.31
1	AA	149	A	C8-N7	8.02	1.37	1.31
1	AA	393	A	C8-N7	8.02	1.37	1.31
22	BA	1175	A	C8-N7	8.01	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1246	A	C8-N7	8.01	1.37	1.31
1	AA	1250	A	C8-N7	8.01	1.37	1.31
22	BA	1095	A	C8-N7	8.01	1.37	1.31
1	AA	1155	A	C8-N7	8.00	1.37	1.31
1	AA	1227	A	C8-N7	8.00	1.37	1.31
1	AA	451	A	C8-N7	7.99	1.37	1.31
22	BA	2564	A	C5-C4	-7.99	1.33	1.38
1	AA	468	A	C8-N7	7.98	1.37	1.31
1	AA	1145	A	C8-N7	7.98	1.37	1.31
22	BA	1505	A	C8-N7	7.98	1.37	1.31
22	BA	899	A	C8-N7	7.97	1.37	1.31
22	BA	2095	A	C8-N7	7.97	1.37	1.31
1	AA	1022	A	C8-N7	7.97	1.37	1.31
22	BA	1069	A	C8-N7	7.97	1.37	1.31
22	BA	1504	A	C8-N7	7.97	1.37	1.31
22	BA	1535	A	C8-N7	7.96	1.37	1.31
1	AA	1318	A	C8-N7	7.96	1.37	1.31
22	BA	1262	A	C5-C4	-7.96	1.33	1.38
22	BA	1090	A	C8-N7	7.96	1.37	1.31
1	AA	1014	A	C8-N7	7.95	1.37	1.31
22	BA	582	A	C5-C4	-7.95	1.33	1.38
1	AA	80	A	C8-N7	7.95	1.37	1.31
22	BA	1413	A	C8-N7	7.95	1.37	1.31
1	AA	197	A	C8-N7	7.94	1.37	1.31
22	BA	878	A	C8-N7	7.94	1.37	1.31
1	AA	143	A	C8-N7	7.94	1.37	1.31
1	AA	1492	A	C8-N7	7.94	1.37	1.31
22	BA	1735	A	C8-N7	7.94	1.37	1.31
1	AA	1251	A	C8-N7	7.93	1.37	1.31
22	BA	2169	A	C8-N7	7.93	1.37	1.31
22	BA	2134	A	C8-N7	7.93	1.37	1.31
1	AA	1216	A	C8-N7	7.93	1.37	1.31
1	AA	1280	A	C8-N7	7.93	1.37	1.31
1	AA	44	A	C8-N7	7.93	1.37	1.31
1	AA	974	A	C8-N7	7.91	1.37	1.31
1	AA	1117	A	C8-N7	7.91	1.37	1.31
22	BA	119	A	C8-N7	7.91	1.37	1.31
22	BA	666	A	C5-C4	-7.90	1.33	1.38
1	AA	415	A	C8-N7	7.90	1.37	1.31
1	AA	456	A	C8-N7	7.90	1.37	1.31
1	AA	872	A	C8-N7	7.89	1.37	1.31
1	AA	435	A	C8-N7	7.89	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	C5-C4	-7.89	1.33	1.38
1	AA	493	A	C8-N7	7.89	1.37	1.31
22	BA	1586	A	C8-N7	7.89	1.37	1.31
22	BA	2449	U	C2-N3	7.89	1.43	1.37
22	BA	2602	A	C8-N7	7.88	1.37	1.31
1	AA	1252	A	C8-N7	7.88	1.37	1.31
1	AA	546	A	C8-N7	7.88	1.37	1.31
22	BA	2135	A	C8-N7	7.88	1.37	1.31
22	BA	1067	A	C8-N7	7.87	1.37	1.31
1	AA	131	A	C8-N7	7.87	1.37	1.31
1	AA	179	A	C8-N7	7.87	1.37	1.31
1	AA	1105	A	C8-N7	7.87	1.37	1.31
22	BA	1515	A	C8-N7	7.87	1.37	1.31
22	BA	2749	A	C8-N7	7.87	1.37	1.31
1	AA	151	A	C8-N7	7.87	1.37	1.31
22	BA	1503	A	C8-N7	7.87	1.37	1.31
1	AA	749	A	C8-N7	7.87	1.37	1.31
1	AA	539	A	C8-N7	7.86	1.37	1.31
22	BA	735	A	C5-C4	-7.86	1.33	1.38
1	AA	889	A	C8-N7	7.86	1.37	1.31
1	AA	1238	A	C8-N7	7.86	1.37	1.31
1	AA	753	A	C8-N7	7.86	1.37	1.31
1	AA	1274	A	C8-N7	7.86	1.37	1.31
22	BA	900	A	C8-N7	7.86	1.37	1.31
1	AA	1333	A	C8-N7	7.86	1.37	1.31
22	BA	2430	A	N9-C4	-7.86	1.33	1.37
22	BA	2469	A	C5-C4	-7.86	1.33	1.38
1	AA	621	A	C8-N7	7.86	1.37	1.31
1	AA	1146	A	C8-N7	7.85	1.37	1.31
22	BA	1096	A	C8-N7	7.85	1.37	1.31
1	AA	1269	A	C8-N7	7.85	1.37	1.31
1	AA	66	A	C8-N7	7.85	1.37	1.31
1	AA	2	A	C8-N7	7.84	1.37	1.31
1	AA	913	A	C8-N7	7.84	1.37	1.31
22	BA	2541	A	C5-C4	-7.84	1.33	1.38
1	AA	845	A	C8-N7	7.84	1.37	1.31
1	AA	1368	A	C8-N7	7.83	1.37	1.31
22	BA	1086	A	C8-N7	7.83	1.37	1.31
1	AA	1035	A	C8-N7	7.83	1.37	1.31
1	AA	71	A	C8-N7	7.83	1.37	1.31
1	AA	704	A	C8-N7	7.83	1.37	1.31
1	AA	129	A	C8-N7	7.82	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	978	A	C8-N7	7.82	1.37	1.31
22	BA	1808	A	C8-N7	7.82	1.37	1.31
22	BA	2381	A	C5-C4	-7.82	1.33	1.38
1	AA	1349	A	C8-N7	7.82	1.37	1.31
22	BA	2753	A	C8-N7	7.82	1.37	1.31
22	BA	1244	A	C5-C4	-7.82	1.33	1.38
1	AA	509	A	C8-N7	7.81	1.37	1.31
1	AA	1456	A	C8-N7	7.81	1.37	1.31
1	AA	1	A	C8-N7	7.81	1.37	1.31
1	AA	60	A	C8-N7	7.81	1.37	1.31
22	BA	1978	A	C5-C4	-7.81	1.33	1.38
1	AA	353	A	C8-N7	7.81	1.37	1.31
1	AA	167	A	C8-N7	7.80	1.37	1.31
1	AA	579	A	C8-N7	7.80	1.37	1.31
22	BA	2094	A	C8-N7	7.80	1.37	1.31
1	AA	139	A	C8-N7	7.80	1.37	1.31
1	AA	1248	A	C8-N7	7.80	1.37	1.31
1	AA	648	A	C8-N7	7.79	1.37	1.31
1	AA	1080	A	C8-N7	7.79	1.37	1.31
1	AA	1311	A	C8-N7	7.79	1.37	1.31
22	BA	1640	A	C5-C4	-7.79	1.33	1.38
1	AA	243	A	C8-N7	7.79	1.37	1.31
22	BA	1566	A	C5-C4	-7.79	1.33	1.38
1	AA	747	A	C8-N7	7.79	1.36	1.31
22	BA	2154	A	C8-N7	7.79	1.36	1.31
1	AA	465	A	C5-C4	-7.78	1.33	1.38
1	AA	1289	A	C8-N7	7.78	1.36	1.31
1	AA	466	A	C8-N7	7.78	1.36	1.31
1	AA	547	A	C8-N7	7.78	1.36	1.31
22	BA	2309	A	C8-N7	7.78	1.36	1.31
1	AA	1410	A	C8-N7	7.78	1.36	1.31
22	BA	1952	A	C5-C4	-7.77	1.33	1.38
1	AA	1169	A	C8-N7	7.77	1.36	1.31
22	BA	896	A	C8-N7	7.77	1.36	1.31
22	BA	2170	A	C8-N7	7.77	1.36	1.31
22	BA	1103	A	C8-N7	7.77	1.36	1.31
1	AA	1180	A	C8-N7	7.76	1.36	1.31
1	AA	72	A	C8-N7	7.76	1.36	1.31
1	AA	959	A	C8-N7	7.76	1.36	1.31
1	AA	441	A	C8-N7	7.76	1.36	1.31
1	AA	572	A	C8-N7	7.76	1.36	1.31
22	BA	556	A	C5-C4	-7.76	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	925	A	C5-C4	-7.76	1.33	1.38
1	AA	77	A	C8-N7	7.75	1.36	1.31
1	AA	600	A	C8-N7	7.75	1.36	1.31
1	AA	482	A	C8-N7	7.75	1.36	1.31
1	AA	1441	A	C8-N7	7.75	1.36	1.31
22	BA	1241	A	C5-C4	-7.75	1.33	1.38
1	AA	374	A	C8-N7	7.75	1.36	1.31
22	BA	1073	A	C8-N7	7.75	1.36	1.31
1	AA	172	A	C8-N7	7.75	1.36	1.31
22	BA	172	A	C8-N7	7.75	1.36	1.31
22	BA	613	A	C8-N7	7.75	1.36	1.31
1	AA	223	A	C8-N7	7.75	1.36	1.31
1	AA	336	A	C8-N7	7.75	1.36	1.31
22	BA	181	A	C8-N7	7.75	1.36	1.31
22	BA	1590	A	C8-N7	7.75	1.36	1.31
1	AA	1152	A	C8-N7	7.74	1.36	1.31
22	BA	56	A	C5-C4	-7.74	1.33	1.38
22	BA	1509	A	C8-N7	7.74	1.36	1.31
22	BA	2126	A	C8-N7	7.74	1.36	1.31
1	AA	363	A	C8-N7	7.73	1.36	1.31
22	BA	2657	A	C8-N7	7.73	1.36	1.31
1	AA	640	A	C8-N7	7.73	1.36	1.31
1	AA	1067	A	C8-N7	7.73	1.36	1.31
1	AA	1201	A	C8-N7	7.72	1.36	1.31
1	AA	8	A	C8-N7	7.72	1.36	1.31
22	BA	272	A	C8-N7	7.72	1.36	1.31
1	AA	532	A	C8-N7	7.72	1.36	1.31
1	AA	969	A	C8-N7	7.72	1.36	1.31
1	AA	1101	A	C8-N7	7.71	1.36	1.31
22	BA	161	A	C8-N7	7.71	1.36	1.31
22	BA	892	A	C8-N7	7.71	1.36	1.31
1	AA	432	A	C8-N7	7.71	1.36	1.31
1	AA	306	A	C8-N7	7.71	1.36	1.31
1	AA	496	A	C8-N7	7.71	1.36	1.31
1	AA	1111	A	C8-N7	7.71	1.36	1.31
22	BA	1495	A	C8-N7	7.71	1.36	1.31
22	BA	1028	A	C5-C4	-7.71	1.33	1.38
22	BA	563	A	C5-C4	-7.70	1.33	1.38
1	AA	595	A	C8-N7	7.70	1.36	1.31
22	BA	342	A	C8-N7	7.70	1.36	1.31
22	BA	470	A	C5-C4	-7.70	1.33	1.38
22	BA	2042	A	C5-C4	-7.69	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1036	A	C8-N7	7.69	1.36	1.31
1	AA	1110	A	C8-N7	7.69	1.36	1.31
22	BA	2163	A	C8-N7	7.68	1.36	1.31
1	AA	949	A	C8-N7	7.67	1.36	1.31
1	AA	994	A	C8-N7	7.67	1.36	1.31
22	BA	532	A	C5-C4	-7.67	1.33	1.38
1	AA	655	A	C8-N7	7.67	1.36	1.31
22	BA	685	A	C5-C4	-7.67	1.33	1.38
22	BA	1304	A	C5-C4	-7.67	1.33	1.38
1	AA	382	A	C8-N7	7.66	1.36	1.31
1	AA	535	A	C8-N7	7.66	1.36	1.31
1	AA	673	A	C8-N7	7.66	1.36	1.31
1	AA	1157	A	C8-N7	7.66	1.36	1.31
22	BA	2809	A	C5-C4	-7.66	1.33	1.38
22	BA	391	A	C5-C4	-7.66	1.33	1.38
1	AA	831	A	C8-N7	7.66	1.36	1.31
1	AA	1285	A	C8-N7	7.66	1.36	1.31
22	BA	2184	A	C8-N7	7.66	1.36	1.31
22	BA	2660	A	C8-N7	7.65	1.36	1.31
1	AA	205	A	C8-N7	7.65	1.36	1.31
1	AA	315	A	C8-N7	7.65	1.36	1.31
1	AA	1176	A	C8-N7	7.65	1.36	1.31
1	AA	1493	A	C8-N7	7.65	1.36	1.31
1	AA	1219	A	C8-N7	7.64	1.36	1.31
1	AA	199	A	C8-N7	7.64	1.36	1.31
1	AA	649	A	C8-N7	7.64	1.36	1.31
1	AA	1092	A	C8-N7	7.64	1.36	1.31
22	BA	1532	A	C8-N7	7.64	1.36	1.31
22	BA	2158	A	C8-N7	7.63	1.36	1.31
22	BA	2530	A	C8-N7	7.63	1.36	1.31
22	BA	2176	A	C8-N7	7.63	1.36	1.31
1	AA	825	A	C8-N7	7.63	1.36	1.31
1	AA	98	A	C8-N7	7.63	1.36	1.31
22	BA	668	A	C5-C4	-7.63	1.33	1.38
22	BA	1970	A	C5-C4	-7.63	1.33	1.38
22	BA	1998	A	C5-C4	-7.63	1.33	1.38
22	BA	1609	A	C5-C4	-7.63	1.33	1.38
22	BA	111	A	C8-N7	7.62	1.36	1.31
1	AA	1093	A	C8-N7	7.62	1.36	1.31
22	BA	142	A	C8-N7	7.62	1.36	1.31
22	BA	917	A	C5-C4	-7.62	1.33	1.38
1	AA	983	A	C8-N7	7.62	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1020	A	C8-N7	7.62	1.36	1.31
22	BA	2600	A	C5-C4	-7.62	1.33	1.38
22	BA	84	A	C5-C4	-7.61	1.33	1.38
22	BA	453	A	C5-C4	-7.61	1.33	1.38
22	BA	2142	A	C8-N7	7.61	1.36	1.31
22	BA	2459	A	C5-C4	-7.61	1.33	1.38
1	AA	282	A	C8-N7	7.61	1.36	1.31
1	AA	495	A	C8-N7	7.61	1.36	1.31
22	BA	1916	A	C8-N7	7.61	1.36	1.31
1	AA	1275	A	C8-N7	7.61	1.36	1.31
1	AA	155	A	C8-N7	7.61	1.36	1.31
22	BA	1508	A	C8-N7	7.61	1.36	1.31
22	BA	160	A	C8-N7	7.60	1.36	1.31
22	BA	1322	A	C5-C4	-7.60	1.33	1.38
22	BA	1913	A	C8-N7	7.60	1.36	1.31
22	BA	2758	A	C8-N7	7.60	1.36	1.31
1	AA	236	A	C8-N7	7.60	1.36	1.31
22	BA	1871	A	C8-N7	7.60	1.36	1.31
22	BA	1205	A	C8-N7	7.59	1.36	1.31
22	BA	2469	A	C8-N7	7.59	1.36	1.31
22	BA	165	A	C8-N7	7.59	1.36	1.31
22	BA	788	A	C5-C4	-7.59	1.33	1.38
22	BA	1392	A	C5-C4	-7.59	1.33	1.38
1	AA	3	A	C8-N7	7.59	1.36	1.31
1	AA	1362	A	C8-N7	7.58	1.36	1.31
22	BA	2738	A	C5-C4	-7.58	1.33	1.38
1	AA	120	A	C8-N7	7.58	1.36	1.31
1	AA	478	A	C8-N7	7.58	1.36	1.31
1	AA	1021	A	C8-N7	7.58	1.36	1.31
22	BA	126	A	C5-C4	-7.58	1.33	1.38
1	AA	935	A	C8-N7	7.58	1.36	1.31
22	BA	1626	A	C5-C4	-7.58	1.33	1.38
22	BA	2020	A	C5-C4	-7.58	1.33	1.38
1	AA	16	A	C8-N7	7.58	1.36	1.31
22	BA	2406	A	C8-N7	7.58	1.36	1.31
1	AA	1225	A	C8-N7	7.57	1.36	1.31
22	BA	362	A	C8-N7	7.57	1.36	1.31
22	BA	905	A	C8-N7	7.57	1.36	1.31
22	BA	608	A	C5-C4	-7.57	1.33	1.38
22	BA	1084	A	C8-N7	7.57	1.36	1.31
1	AA	263	A	C8-N7	7.57	1.36	1.31
1	AA	1271	A	C8-N7	7.57	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	609	A	C8-N7	7.57	1.36	1.31
22	BA	2054	A	C5-C4	-7.57	1.33	1.38
1	AA	1171	A	C8-N7	7.56	1.36	1.31
22	BA	1705	A	C5-C4	-7.56	1.33	1.38
1	AA	1167	A	C8-N7	7.56	1.36	1.31
1	AA	101	A	C8-N7	7.55	1.36	1.31
1	AA	279	A	C8-N7	7.55	1.36	1.31
1	AA	7	A	C8-N7	7.55	1.36	1.31
1	AA	174	A	C8-N7	7.55	1.36	1.31
22	BA	1039	A	C8-N7	7.55	1.36	1.31
55	B8	76	A	C5-C4	-7.54	1.33	1.38
1	AA	1350	A	C8-N7	7.54	1.36	1.31
22	BA	1960	A	C5-C4	-7.54	1.33	1.38
22	BA	1427	A	C8-N7	7.54	1.36	1.31
1	AA	766	A	C8-N7	7.54	1.36	1.31
1	AA	262	A	C8-N7	7.54	1.36	1.31
1	AA	411	A	C8-N7	7.54	1.36	1.31
22	BA	541	A	C5-C4	-7.53	1.33	1.38
1	AA	1256	A	C8-N7	7.52	1.36	1.31
22	BA	1652	A	C5-C4	-7.52	1.33	1.38
22	BA	347	A	C8-N7	7.51	1.36	1.31
22	BA	2761	A	C8-N7	7.51	1.36	1.31
22	BA	910	A	C5-C4	-7.51	1.33	1.38
1	AA	675	A	C8-N7	7.51	1.36	1.31
22	BA	330	A	C5-C4	-7.51	1.33	1.38
1	AA	583	A	C8-N7	7.51	1.36	1.31
22	BA	197	A	C5-C4	-7.51	1.33	1.38
1	AA	777	A	C8-N7	7.51	1.36	1.31
22	BA	299	A	C5-C4	-7.51	1.33	1.38
22	BA	2183	A	C8-N7	7.51	1.36	1.31
22	BA	572	A	C5-C4	-7.50	1.33	1.38
1	AA	487	A	C8-N7	7.50	1.36	1.31
1	AA	1254	A	C8-N7	7.50	1.36	1.31
1	AA	510	A	C8-N7	7.50	1.36	1.31
1	AA	975	A	C8-N7	7.50	1.36	1.31
22	BA	282	A	C8-N7	7.50	1.36	1.31
22	BA	1966	A	C5-C4	-7.50	1.33	1.38
1	AA	1468	A	C5-C4	-7.49	1.33	1.38
1	AA	430	A	C8-N7	7.49	1.36	1.31
1	AA	523	A	C8-N7	7.49	1.36	1.31
22	BA	1054	A	C8-N7	7.49	1.36	1.31
22	BA	794	A	C5-C4	-7.49	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	607	A	C8-N7	7.49	1.36	1.31
22	BA	368	A	C8-N7	7.48	1.36	1.31
22	BA	716	A	C8-N7	7.48	1.36	1.31
22	BA	1932	A	C5-C4	-7.48	1.33	1.38
1	AA	1191	A	C8-N7	7.48	1.36	1.31
22	BA	1048	A	C8-N7	7.48	1.36	1.31
22	BA	750	A	C5-C4	-7.48	1.33	1.38
1	AA	309	A	C8-N7	7.48	1.36	1.31
22	BA	1027	A	C5-C4	-7.48	1.33	1.38
22	BA	2060	A	C5-C4	-7.47	1.33	1.38
1	AA	1363	A	C8-N7	7.47	1.36	1.31
22	BA	155	A	C8-N7	7.47	1.36	1.31
1	AA	602	A	C8-N7	7.47	1.36	1.31
22	BA	2013	A	C5-C4	-7.47	1.33	1.38
1	AA	499	A	C8-N7	7.47	1.36	1.31
1	AA	687	A	C8-N7	7.47	1.36	1.31
22	BA	195	A	C8-N7	7.47	1.36	1.31
22	BA	508	A	C8-N7	7.46	1.36	1.31
22	BA	972	A	C5-C4	-7.46	1.33	1.38
1	AA	1480	A	C8-N7	7.46	1.36	1.31
22	BA	1593	A	C8-N7	7.46	1.36	1.31
22	BA	911	A	C5-C4	-7.46	1.33	1.38
1	AA	228	A	C8-N7	7.46	1.36	1.31
22	BA	670	A	C5-C4	-7.46	1.33	1.38
22	BA	1272	A	C5-C4	-7.46	1.33	1.38
1	AA	792	A	C5-C4	-7.46	1.33	1.38
13	AM	115	PRO	N-CA	-7.46	1.34	1.47
22	BA	84	A	C8-N7	7.45	1.36	1.31
22	BA	2108	A	C8-N7	7.45	1.36	1.31
1	AA	78	A	C8-N7	7.45	1.36	1.31
1	AA	681	A	C8-N7	7.45	1.36	1.31
1	AA	918	A	C8-N7	7.45	1.36	1.31
22	BA	1490	A	C8-N7	7.45	1.36	1.31
22	BA	2670	A	C5-C4	-7.45	1.33	1.38
1	AA	1196	A	C8-N7	7.45	1.36	1.31
1	AA	130	A	C8-N7	7.44	1.36	1.31
1	AA	815	A	C8-N7	7.44	1.36	1.31
22	BA	2311	A	C8-N7	7.44	1.36	1.31
22	BA	2654	A	C8-N7	7.44	1.36	1.31
1	AA	274	A	C5-C4	-7.44	1.33	1.38
1	AA	238	A	C8-N7	7.44	1.36	1.31
1	AA	1319	A	C5-C4	-7.44	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1040	A	C8-N7	7.44	1.36	1.31
22	BA	1672	A	C5-C4	-7.43	1.33	1.38
1	AA	767	A	C5-C4	-7.43	1.33	1.38
1	AA	1102	A	C8-N7	7.43	1.36	1.31
1	AA	321	A	C8-N7	7.42	1.36	1.31
1	AA	1434	A	C8-N7	7.42	1.36	1.31
1	AA	270	A	C8-N7	7.42	1.36	1.31
22	BA	344	A	C8-N7	7.42	1.36	1.31
1	AA	1046	A	C8-N7	7.42	1.36	1.31
22	BA	1354	A	C5-C4	-7.42	1.33	1.38
22	BA	1085	A	C8-N7	7.42	1.36	1.31
22	BA	1717	A	C8-N7	7.42	1.36	1.31
1	AA	919	A	C8-N7	7.41	1.36	1.31
1	AA	676	A	C8-N7	7.41	1.36	1.31
22	BA	2314	A	C8-N7	7.41	1.36	1.31
22	BA	2435	A	C5-C4	-7.41	1.33	1.38
23	BB	15	A	C8-N7	7.41	1.36	1.31
22	BA	1419	A	C8-N7	7.41	1.36	1.31
22	BA	2377	A	C5-C4	-7.41	1.33	1.38
1	AA	729	A	C8-N7	7.41	1.36	1.31
22	BA	1580	A	C8-N7	7.40	1.36	1.31
22	BA	2376	A	C5-C4	-7.40	1.33	1.38
23	BB	104	A	C5-C4	-7.40	1.33	1.38
1	AA	119	A	C8-N7	7.40	1.36	1.31
22	BA	654	A	C8-N7	7.40	1.36	1.31
1	AA	181	A	C8-N7	7.39	1.36	1.31
1	AA	1531	A	C8-N7	7.39	1.36	1.31
1	AA	1413	A	C8-N7	7.39	1.36	1.31
23	BB	53	A	C8-N7	7.39	1.36	1.31
1	AA	909	A	C8-N7	7.39	1.36	1.31
1	AA	663	A	C8-N7	7.39	1.36	1.31
1	AA	1340	A	C5-C4	-7.39	1.33	1.38
1	AA	1374	A	C8-N7	7.39	1.36	1.31
22	BA	1151	A	C5-C4	-7.39	1.33	1.38
23	BB	66	A	C8-N7	7.39	1.36	1.31
1	AA	364	A	C8-N7	7.38	1.36	1.31
22	BA	1194	A	C5-C4	-7.38	1.33	1.38
1	AA	635	A	C8-N7	7.38	1.36	1.31
22	BA	255	A	C5-C4	-7.38	1.33	1.38
22	BA	1453	A	C8-N7	7.38	1.36	1.31
22	BA	504	A	C8-N7	7.38	1.36	1.31
1	AA	344	A	C8-N7	7.38	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	262	A	C5-C4	-7.38	1.33	1.38
23	BB	34	A	C8-N7	7.38	1.36	1.31
22	BA	2800	A	C8-N7	7.37	1.36	1.31
22	BA	1000	A	C5-C4	-7.37	1.33	1.38
1	AA	1324	A	C8-N7	7.37	1.36	1.31
22	BA	5	A	C8-N7	7.37	1.36	1.31
22	BA	2635	A	C5-C4	-7.37	1.33	1.38
22	BA	213	A	C8-N7	7.36	1.36	1.31
22	BA	693	A	C5-C4	-7.36	1.33	1.38
22	BA	1287	A	C5-C4	-7.36	1.33	1.38
1	AA	349	A	C8-N7	7.35	1.36	1.31
1	AA	298	A	C8-N7	7.35	1.36	1.31
25	BD	152	PRO	N-CA	-7.35	1.34	1.47
1	AA	878	A	C8-N7	7.35	1.36	1.31
1	AA	325	A	C8-N7	7.35	1.36	1.31
1	AA	1236	A	C8-N7	7.35	1.36	1.31
22	BA	270	A	C8-N7	7.35	1.36	1.31
1	AA	246	A	C8-N7	7.34	1.36	1.31
1	AA	1082	A	C8-N7	7.34	1.36	1.31
22	BA	2471	A	C5-C4	-7.34	1.33	1.38
1	AA	448	A	C8-N7	7.34	1.36	1.31
1	AA	712	A	C8-N7	7.34	1.36	1.31
22	BA	415	A	C5-C4	-7.34	1.33	1.38
22	BA	1502	A	C8-N7	7.34	1.36	1.31
22	BA	1549	A	C5-C4	-7.34	1.33	1.38
1	AA	465	A	C8-N7	7.33	1.36	1.31
1	AA	1507	A	C8-N7	7.33	1.36	1.31
22	BA	309	A	C5-C4	-7.33	1.33	1.38
22	BA	2542	A	C5-C4	-7.33	1.33	1.38
22	BA	1889	A	C8-N7	7.33	1.36	1.31
1	AA	303	A	C8-N7	7.33	1.36	1.31
22	BA	278	A	C8-N7	7.33	1.36	1.31
22	BA	2750	A	C8-N7	7.33	1.36	1.31
23	BB	115	A	C8-N7	7.32	1.36	1.31
22	BA	348	A	C8-N7	7.32	1.36	1.31
22	BA	1156	A	C5-C4	-7.32	1.33	1.38
22	BA	1596	A	C8-N7	7.32	1.36	1.31
1	AA	1513	A	C8-N7	7.32	1.36	1.31
1	AA	327	A	C8-N7	7.32	1.36	1.31
22	BA	909	A	C5-C4	-7.32	1.33	1.38
22	BA	2781	A	C5-C4	-7.32	1.33	1.38
1	AA	946	A	C8-N7	7.32	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	715	A	C8-N7	7.32	1.36	1.31
22	BA	2482	A	C5-C4	-7.32	1.33	1.38
1	AA	1375	A	C8-N7	7.31	1.36	1.31
22	BA	825	A	C5-C4	-7.31	1.33	1.38
22	BA	996	A	C5-C4	-7.31	1.33	1.38
22	BA	1169	A	C8-N7	7.31	1.36	1.31
22	BA	1383	A	C8-N7	7.31	1.36	1.31
22	BA	507	A	C8-N7	7.31	1.36	1.31
22	BA	1264	A	C5-C4	-7.31	1.33	1.38
22	BA	213	A	C5-C4	-7.31	1.33	1.38
22	BA	2173	A	C8-N7	7.31	1.36	1.31
22	BA	2468	A	C5-C4	-7.31	1.33	1.38
22	BA	2900	A	C8-N7	7.31	1.36	1.31
1	AA	250	A	C8-N7	7.31	1.36	1.31
1	AA	461	A	N3-C4	7.30	1.39	1.34
1	AA	1398	A	C8-N7	7.30	1.36	1.31
22	BA	199	A	C5-C4	-7.30	1.33	1.38
22	BA	1821	A	C5-C4	-7.30	1.33	1.38
22	BA	2792	A	C8-N7	7.30	1.36	1.31
22	BA	223	A	C5-C4	-7.30	1.33	1.38
1	AA	1306	A	C8-N7	7.29	1.36	1.31
1	AA	1163	A	C8-N7	7.29	1.36	1.31
22	BA	632	A	C5-C4	-7.29	1.33	1.38
22	BA	1858	A	C5-C4	-7.29	1.33	1.38
1	AA	313	A	C8-N7	7.29	1.36	1.31
22	BA	2003	A	C5-C4	-7.29	1.33	1.38
1	AA	65	A	C8-N7	7.29	1.36	1.31
1	AA	642	A	C8-N7	7.29	1.36	1.31
22	BA	721	A	C8-N7	7.28	1.36	1.31
22	BA	792	A	C5-C4	-7.28	1.33	1.38
22	BA	1591	A	C8-N7	7.28	1.36	1.31
1	AA	728	A	C8-N7	7.28	1.36	1.31
1	AA	706	A	C8-N7	7.28	1.36	1.31
22	BA	2453	A	C5-C4	-7.28	1.33	1.38
22	BA	2700	A	C5-C4	-7.28	1.33	1.38
22	BA	793	A	C5-C4	-7.27	1.33	1.38
22	BA	1749	A	C8-N7	7.27	1.36	1.31
22	BA	1098	A	C8-N7	7.27	1.36	1.31
22	BA	1579	A	C8-N7	7.27	1.36	1.31
22	BA	1494	A	C8-N7	7.27	1.36	1.31
22	BA	1759	A	C5-C4	-7.27	1.33	1.38
22	BA	1762	A	C5-C4	-7.27	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2748	A	C8-N7	7.27	1.36	1.31
1	AA	109	A	C8-N7	7.26	1.36	1.31
1	AA	160	A	C8-N7	7.26	1.36	1.31
22	BA	1936	A	C5-C4	-7.26	1.33	1.38
1	AA	1261	A	C8-N7	7.26	1.36	1.31
22	BA	1632	A	C5-C4	-7.26	1.33	1.38
1	AA	1229	A	C8-N7	7.26	1.36	1.31
22	BA	2198	A	C8-N7	7.26	1.36	1.31
1	AA	964	A	C8-N7	7.26	1.36	1.31
22	BA	599	A	C5-C4	-7.25	1.33	1.38
22	BA	727	A	C5-C4	-7.25	1.33	1.38
1	AA	553	A	C8-N7	7.25	1.36	1.31
22	BA	2764	A	C8-N7	7.25	1.36	1.31
22	BA	460	A	C5-C4	-7.25	1.33	1.38
22	BA	2433	A	C5-C4	-7.25	1.33	1.38
22	BA	2670	A	C8-N7	7.25	1.36	1.31
22	BA	222	A	C5-C4	-7.25	1.33	1.38
22	BA	227	A	C5-C4	-7.24	1.33	1.38
22	BA	609	A	C5-C4	-7.24	1.33	1.38
23	BB	58	A	C8-N7	7.24	1.36	1.31
1	AA	694	A	C8-N7	7.24	1.36	1.31
22	BA	44	A	C8-N7	7.24	1.36	1.31
1	AA	320	A	C8-N7	7.24	1.36	1.31
1	AA	915	A	C8-N7	7.24	1.36	1.31
1	AA	502	A	C8-N7	7.24	1.36	1.31
1	AA	608	A	C8-N7	7.24	1.36	1.31
22	BA	1285	A	C8-N7	7.24	1.36	1.31
22	BA	176	A	C5-C4	-7.23	1.33	1.38
22	BA	1342	A	C5-C4	-7.23	1.33	1.38
22	BA	643	A	C5-C4	-7.23	1.33	1.38
22	BA	1496	A	C8-N7	7.23	1.36	1.31
22	BA	734	A	C5-C4	-7.23	1.33	1.38
22	BA	1722	A	C8-N7	7.23	1.36	1.31
22	BA	1809	A	C5-C4	-7.23	1.33	1.38
1	AA	26	A	C8-N7	7.23	1.36	1.31
22	BA	1570	A	C5-C4	-7.23	1.33	1.38
22	BA	1111	A	C8-N7	7.23	1.36	1.31
1	AA	702	A	C8-N7	7.22	1.36	1.31
23	BB	45	A	C8-N7	7.22	1.36	1.31
1	AA	1055	A	C8-N7	7.22	1.36	1.31
22	BA	94	A	C8-N7	7.22	1.36	1.31
22	BA	2879	A	C5-C4	-7.22	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	784	A	C8-N7	7.22	1.36	1.31
1	AA	860	A	C8-N7	7.22	1.36	1.31
1	AA	1012	A	C8-N7	7.22	1.36	1.31
22	BA	1938	A	C5-C4	-7.22	1.33	1.38
22	BA	2534	A	C8-N7	7.22	1.36	1.31
22	BA	621	A	C8-N7	7.21	1.36	1.31
22	BA	2033	A	C8-N7	7.21	1.36	1.31
1	AA	19	A	C8-N7	7.21	1.36	1.31
22	BA	984	A	C5-C4	-7.21	1.33	1.38
1	AA	59	A	C8-N7	7.21	1.36	1.31
22	BA	19	A	C5-C4	-7.21	1.33	1.38
22	BA	730	A	C5-C4	-7.21	1.33	1.38
22	BA	1866	A	C8-N7	7.21	1.36	1.31
22	BA	2009	A	C5-C4	-7.20	1.33	1.38
22	BA	2726	A	C8-N7	7.20	1.36	1.31
1	AA	596	A	C8-N7	7.20	1.36	1.31
22	BA	575	A	C5-C4	-7.20	1.33	1.38
1	AA	937	A	C8-N7	7.20	1.36	1.31
1	AA	50	A	C8-N7	7.20	1.36	1.31
1	AA	782	A	C8-N7	7.20	1.36	1.31
22	BA	2317	A	C8-N7	7.20	1.36	1.31
22	BA	322	A	C8-N7	7.19	1.36	1.31
22	BA	439	A	C8-N7	7.19	1.36	1.31
22	BA	454	A	C8-N7	7.19	1.36	1.31
1	AA	10	A	C8-N7	7.19	1.36	1.31
22	BA	207	A	C5-C4	-7.19	1.33	1.38
22	BA	2471	A	C8-N7	7.19	1.36	1.31
23	BB	46	A	C8-N7	7.19	1.36	1.31
23	BB	108	A	C8-N7	7.19	1.36	1.31
22	BA	404	A	C8-N7	7.19	1.36	1.31
1	AA	51	A	C8-N7	7.18	1.36	1.31
22	BA	592	A	C5-C4	-7.18	1.33	1.38
22	BA	603	A	C8-N7	7.18	1.36	1.31
22	BA	866	A	C5-C4	-7.18	1.33	1.38
22	BA	1155	A	C5-C4	-7.18	1.33	1.38
22	BA	1690	A	C5-C4	-7.18	1.33	1.38
22	BA	2679	A	C5-C4	-7.18	1.33	1.38
22	BA	603	A	C5-C4	-7.18	1.33	1.38
22	BA	2572	A	C5-C4	-7.18	1.33	1.38
22	BA	324	A	C5-C4	-7.18	1.33	1.38
22	BA	382	A	C5-C4	-7.18	1.33	1.38
1	AA	906	A	C8-N7	7.17	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	752	A	C8-N7	7.17	1.36	1.31
22	BA	2058	A	C5-C4	-7.17	1.33	1.38
22	BA	676	A	C5-C4	-7.17	1.33	1.38
23	BB	109	A	C8-N7	7.17	1.36	1.31
1	AA	560	A	C8-N7	7.17	1.36	1.31
22	BA	2090	A	C5-C4	-7.17	1.33	1.38
22	BA	2820	A	C8-N7	7.16	1.36	1.31
22	BA	1794	A	C5-C4	-7.16	1.33	1.38
22	BA	644	A	C5-C4	-7.16	1.33	1.38
22	BA	1987	A	C5-C4	-7.16	1.33	1.38
22	BA	2675	A	C5-C4	-7.16	1.33	1.38
22	BA	2821	A	C5-C4	-7.16	1.33	1.38
22	BA	2835	A	C5-C4	-7.16	1.33	1.38
1	AA	338	A	C8-N7	7.16	1.36	1.31
1	AA	1396	A	C8-N7	7.16	1.36	1.31
1	AA	161	A	C8-N7	7.15	1.36	1.31
22	BA	2740	A	C5-C4	-7.15	1.33	1.38
22	BA	2478	A	C5-C4	-7.15	1.33	1.38
22	BA	1789	A	C5-C4	-7.15	1.33	1.38
22	BA	1088	A	C8-N7	7.15	1.36	1.31
22	BA	1664	A	C5-C4	-7.15	1.33	1.38
22	BA	2097	A	C8-N7	7.15	1.36	1.31
22	BA	2059	A	C8-N7	7.14	1.36	1.31
22	BA	2736	A	C8-N7	7.14	1.36	1.31
1	AA	411	A	C5-C4	-7.14	1.33	1.38
1	AA	629	A	C8-N7	7.14	1.36	1.31
22	BA	614	A	C8-N7	7.14	1.36	1.31
22	BA	346	A	C8-N7	7.14	1.36	1.31
22	BA	1419	A	C5-C4	-7.14	1.33	1.38
22	BA	1129	A	C5-C4	-7.14	1.33	1.38
22	BA	2080	A	C5-C4	-7.14	1.33	1.38
1	AA	968	A	C8-N7	7.13	1.36	1.31
1	AA	923	A	C8-N7	7.13	1.36	1.31
22	BA	1755	A	C5-C4	-7.13	1.33	1.38
22	BA	1230	A	C5-C4	-7.13	1.33	1.38
22	BA	1754	A	N3-C4	7.13	1.39	1.34
22	BA	146	A	C8-N7	7.13	1.36	1.31
22	BA	1885	A	C8-N7	7.12	1.36	1.31
22	BA	2451	A	N3-C4	7.12	1.39	1.34
22	BA	1918	A	C8-N7	7.12	1.36	1.31
22	BA	423	A	C8-N7	7.12	1.36	1.31
22	BA	637	A	C8-N7	7.12	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	28	A	C5-C4	-7.11	1.33	1.38
22	BA	1525	A	C5-C4	-7.11	1.33	1.38
22	BA	2899	A	C8-N7	7.11	1.36	1.31
22	BA	920	A	C5-C4	-7.11	1.33	1.38
22	BA	1805	A	C5-C4	-7.11	1.33	1.38
22	BA	1858	A	C8-N7	7.11	1.36	1.31
22	BA	749	A	C5-C4	-7.11	1.33	1.38
1	AA	1408	A	C8-N7	7.11	1.36	1.31
22	BA	2634	A	C5-C4	-7.11	1.33	1.38
22	BA	1378	A	C5-C4	-7.10	1.33	1.38
1	AA	1394	A	C8-N7	7.10	1.36	1.31
23	BB	50	A	C8-N7	7.10	1.36	1.31
1	AA	1508	A	C8-N7	7.10	1.36	1.31
22	BA	231	A	C5-C4	-7.10	1.33	1.38
22	BA	742	A	C5-C4	-7.10	1.33	1.38
22	BA	1635	A	C5-C4	-7.10	1.33	1.38
1	AA	28	A	C8-N7	7.10	1.36	1.31
22	BA	789	A	C5-C4	-7.10	1.33	1.38
22	BA	1359	A	C5-C4	-7.10	1.33	1.38
23	BB	73	A	C5-C4	-7.10	1.33	1.38
22	BA	980	A	C5-C4	-7.10	1.33	1.38
22	BA	144	A	C5-C4	-7.09	1.33	1.38
1	AA	630	A	C8-N7	7.09	1.36	1.31
22	BA	2346	A	C8-N7	7.09	1.36	1.31
1	AA	787	A	C5-C4	-7.09	1.33	1.38
1	AA	766	A	C5-C4	-7.09	1.33	1.38
22	BA	1544	A	C8-N7	7.09	1.36	1.31
22	BA	513	A	C5-C4	-7.09	1.33	1.38
1	AA	1476	A	C8-N7	7.08	1.36	1.31
22	BA	1308	A	C5-C4	-7.08	1.33	1.38
22	BA	1403	A	C5-C4	-7.08	1.33	1.38
22	BA	1912	A	C8-N7	7.08	1.36	1.31
23	BB	78	A	C5-C4	-7.08	1.33	1.38
22	BA	457	A	C8-N7	7.08	1.36	1.31
22	BA	1384	A	C8-N7	7.08	1.36	1.31
22	BA	1919	A	C8-N7	7.08	1.36	1.31
22	BA	1977	A	C5-C4	-7.08	1.33	1.38
1	AA	718	A	C8-N7	7.08	1.36	1.31
22	BA	472	A	C5-C4	-7.08	1.33	1.38
22	BA	529	A	C8-N7	7.08	1.36	1.31
22	BA	204	A	C5-C4	-7.08	1.33	1.38
1	AA	32	A	C8-N7	7.07	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	116	A	C8-N7	7.07	1.36	1.31
22	BA	933	A	C5-C4	-7.07	1.33	1.38
22	BA	1000	A	C8-N7	7.07	1.36	1.31
1	AA	1430	A	C5-C4	-7.07	1.33	1.38
23	BB	94	A	C5-C4	-7.07	1.33	1.38
1	AA	792	A	C8-N7	7.06	1.36	1.31
22	BA	479	A	C5-C4	-7.06	1.33	1.38
22	BA	1877	A	C8-N7	7.06	1.36	1.31
22	BA	1787	A	C5-C4	-7.06	1.33	1.38
22	BA	1014	A	C8-N7	7.06	1.36	1.31
22	BA	1815	A	C5-C4	-7.06	1.33	1.38
22	BA	294	A	C8-N7	7.06	1.36	1.31
22	BA	2439	A	C8-N7	7.06	1.36	1.31
1	AA	1437	A	C8-N7	7.05	1.36	1.31
22	BA	144	A	C8-N7	7.05	1.36	1.31
22	BA	1522	A	C8-N7	7.05	1.36	1.31
22	BA	1545	A	C8-N7	7.05	1.36	1.31
22	BA	2392	A	C5-C4	-7.05	1.33	1.38
22	BA	2727	A	C5-C4	-7.05	1.33	1.38
1	AA	695	A	C8-N7	7.05	1.36	1.31
22	BA	2566	A	C8-N7	7.05	1.36	1.31
1	AA	977	A	C8-N7	7.05	1.36	1.31
22	BA	1246	A	C8-N7	7.05	1.36	1.31
22	BA	718	A	C8-N7	7.05	1.36	1.31
22	BA	1571	A	C5-C4	-7.05	1.33	1.38
1	AA	253	A	C5-C4	-7.04	1.33	1.38
22	BA	1548	A	C5-C4	-7.04	1.33	1.38
22	BA	1786	A	C5-C4	-7.04	1.33	1.38
1	AA	573	A	C8-N7	7.04	1.36	1.31
22	BA	2340	A	C5-C4	-7.04	1.33	1.38
1	AA	1502	A	C8-N7	7.04	1.36	1.31
22	BA	941	A	C5-C4	-7.04	1.33	1.38
22	BA	1829	A	C5-C4	-7.04	1.33	1.38
22	BA	1328	A	C5-C4	-7.04	1.33	1.38
22	BA	1321	A	C8-N7	7.04	1.36	1.31
22	BA	1655	A	C5-C4	-7.04	1.33	1.38
23	BB	39	A	C8-N7	7.03	1.36	1.31
1	AA	53	A	C8-N7	7.03	1.36	1.31
22	BA	614	A	C5-C4	-7.03	1.33	1.38
1	AA	313	A	C5-C4	-7.03	1.33	1.38
22	BA	221	A	C8-N7	7.03	1.36	1.31
22	BA	443	A	C5-C4	-7.03	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	432	A	C5-C4	-7.03	1.33	1.38
22	BA	384	A	C5-C4	-7.02	1.33	1.38
22	BA	1876	A	C8-N7	7.02	1.36	1.31
22	BA	2212	A	C8-N7	7.02	1.36	1.31
22	BA	156	A	C8-N7	7.02	1.36	1.31
22	BA	936	A	C5-C4	-7.02	1.33	1.38
22	BA	2893	A	C5-C4	-7.02	1.33	1.38
1	AA	19	A	C5-C4	-7.02	1.33	1.38
22	BA	146	A	C5-C4	-7.02	1.33	1.38
22	BA	2632	A	C5-C4	-7.02	1.33	1.38
22	BA	2114	A	C8-N7	7.02	1.36	1.31
22	BA	2358	A	C5-C4	-7.02	1.33	1.38
22	BA	196	A	C5-C4	-7.01	1.33	1.38
22	BA	945	A	C8-N7	7.01	1.36	1.31
22	BA	1347	A	C5-C4	-7.01	1.33	1.38
22	BA	428	A	C5-C4	-7.01	1.33	1.38
22	BA	2531	A	C8-N7	7.01	1.36	1.31
1	AA	759	A	C8-N7	7.01	1.36	1.31
22	BA	2899	A	C5-C4	-7.00	1.33	1.38
22	BA	125	A	C8-N7	7.00	1.36	1.31
55	B8	58	A	C8-N7	7.00	1.36	1.31
22	BA	104	A	C8-N7	7.00	1.36	1.31
22	BA	89	A	C8-N7	7.00	1.36	1.31
22	BA	1383	A	C5-C4	-7.00	1.33	1.38
23	BB	29	A	C8-N7	7.00	1.36	1.31
22	BA	947	A	C5-C4	-7.00	1.33	1.38
22	BA	300	A	C5-C4	-6.99	1.33	1.38
22	BA	1801	A	C5-C4	-6.99	1.33	1.38
22	BA	213	A	N3-C4	6.99	1.39	1.34
22	BA	219	A	C5-C4	-6.99	1.33	1.38
22	BA	905	A	C5-C4	-6.99	1.33	1.38
22	BA	1032	A	C8-N7	6.99	1.36	1.31
22	BA	2733	A	C8-N7	6.99	1.36	1.31
22	BA	2019	A	C5-C4	-6.98	1.33	1.38
1	AA	1035	A	N3-C4	6.98	1.39	1.34
22	BA	2418	A	C5-C4	-6.98	1.33	1.38
22	BA	42	A	C8-N7	6.98	1.36	1.31
23	BB	52	A	C8-N7	6.98	1.36	1.31
22	BA	2518	A	C5-C4	-6.98	1.33	1.38
55	B8	51	A	C8-N7	6.98	1.36	1.31
1	AA	892	A	C5-C4	-6.98	1.33	1.38
22	BA	439	A	C5-C4	-6.97	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1713	A	C8-N7	6.97	1.36	1.31
22	BA	2547	A	C8-N7	6.97	1.36	1.31
22	BA	1650	A	C5-C4	-6.97	1.33	1.38
22	BA	1268	A	C5-C4	-6.97	1.33	1.38
1	AA	1339	A	C5-C4	-6.96	1.33	1.38
22	BA	743	A	C5-C4	-6.96	1.33	1.38
22	BA	761	A	C8-N7	6.96	1.36	1.31
22	BA	2882	A	C8-N7	6.96	1.36	1.31
22	BA	2589	A	C5-C4	-6.96	1.33	1.38
22	BA	973	A	C8-N7	6.96	1.36	1.31
22	BA	1885	A	C5-C4	-6.96	1.33	1.38
22	BA	1569	A	C5-C4	-6.96	1.33	1.38
1	AA	303	A	C5-C4	-6.96	1.33	1.38
22	BA	655	A	C8-N7	6.95	1.36	1.31
1	AA	288	A	C8-N7	6.95	1.36	1.31
22	BA	1385	A	C5-C4	-6.95	1.33	1.38
22	BA	2366	A	C5-C4	-6.95	1.33	1.38
1	AA	559	A	C8-N7	6.95	1.36	1.31
22	BA	1630	A	C8-N7	6.95	1.36	1.31
22	BA	125	A	C5-C4	-6.94	1.33	1.38
22	BA	631	A	C5-C4	-6.94	1.33	1.38
1	AA	938	A	C8-N7	6.94	1.36	1.31
22	BA	340	A	C8-N7	6.94	1.36	1.31
1	AA	864	A	C8-N7	6.94	1.36	1.31
22	BA	74	A	C8-N7	6.94	1.36	1.31
22	BA	119	A	C5-C4	-6.94	1.33	1.38
1	AA	900	A	C5-C4	-6.94	1.33	1.38
22	BA	1247	A	C5-C4	-6.94	1.33	1.38
22	BA	1367	A	C5-C4	-6.94	1.33	1.38
22	BA	1803	A	C5-C4	-6.94	1.33	1.38
1	AA	787	A	C8-N7	6.93	1.36	1.31
22	BA	1284	A	C5-C4	-6.93	1.33	1.38
22	BA	1286	A	C5-C4	-6.93	1.33	1.38
22	BA	1810	A	N7-C5	-6.93	1.35	1.39
22	BA	1392	A	C8-N7	6.93	1.36	1.31
1	AA	498	A	N3-C4	6.93	1.39	1.34
1	AA	1503	A	C8-N7	6.93	1.36	1.31
22	BA	241	A	C8-N7	6.93	1.36	1.31
22	BA	722	A	C5-C4	-6.93	1.33	1.38
22	BA	322	A	C5-C4	-6.93	1.33	1.38
22	BA	2893	A	C8-N7	6.93	1.36	1.31
22	BA	2856	A	C8-N7	6.93	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	746	A	C8-N7	6.92	1.36	1.31
22	BA	1525	A	C8-N7	6.92	1.36	1.31
22	BA	1144	A	C5-C4	-6.92	1.33	1.38
22	BA	1353	A	C8-N7	6.92	1.36	1.31
22	BA	2835	A	C8-N7	6.92	1.36	1.31
1	AA	373	A	C8-N7	6.92	1.36	1.31
1	AA	908	A	C8-N7	6.92	1.36	1.31
22	BA	2287	A	C5-C4	-6.92	1.33	1.38
22	BA	221	A	C5-C4	-6.92	1.33	1.38
22	BA	501	A	C5-C4	-6.92	1.33	1.38
1	AA	7	A	C5-C4	-6.91	1.33	1.38
22	BA	661	A	C5-C4	-6.91	1.33	1.38
22	BA	1213	A	C5-C4	-6.91	1.33	1.38
55	B8	42	A	C8-N7	6.91	1.36	1.31
1	AA	873	A	C5-C4	-6.91	1.33	1.38
22	BA	2052	A	C5-C4	-6.91	1.33	1.38
22	BA	111	A	C5-C4	-6.91	1.33	1.38
22	BA	1515	A	C5-C4	-6.91	1.33	1.38
1	AA	356	A	C8-N7	6.91	1.36	1.31
22	BA	1927	A	C8-N7	6.91	1.36	1.31
22	BA	2476	A	C8-N7	6.91	1.36	1.31
1	AA	498	A	C8-N7	6.91	1.36	1.31
22	BA	1654	A	C5-C4	-6.91	1.33	1.38
22	BA	2823	A	C5-C4	-6.91	1.33	1.38
22	BA	2225	A	C5-C4	-6.90	1.33	1.38
22	BA	1711	A	C5-C4	-6.90	1.33	1.38
23	BB	115	A	C5-C4	-6.90	1.33	1.38
22	BA	161	A	C5-C4	-6.90	1.33	1.38
22	BA	626	A	C8-N7	6.90	1.36	1.31
1	AA	1197	A	C8-N7	6.89	1.36	1.31
22	BA	233	A	C5-C4	-6.89	1.33	1.38
22	BA	1204	A	C8-N7	6.89	1.36	1.31
22	BA	2070	A	C5-C4	-6.89	1.33	1.38
22	BA	2851	A	C5-C4	-6.89	1.33	1.38
22	BA	2736	A	C5-C4	-6.89	1.33	1.38
22	BA	2799	A	N3-C4	6.89	1.39	1.34
1	AA	1357	A	C8-N7	6.89	1.36	1.31
22	BA	621	A	C5-C4	-6.89	1.33	1.38
22	BA	2725	A	C5-C4	-6.89	1.33	1.38
22	BA	574	A	C8-N7	6.88	1.36	1.31
22	BA	721	A	C5-C4	-6.88	1.33	1.38
1	AA	1476	A	C5-C4	-6.88	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	538	A	C5-C4	-6.88	1.33	1.38
22	BA	471	A	C5-C4	-6.88	1.33	1.38
22	BA	1597	A	C8-N7	6.88	1.36	1.31
22	BA	1676	A	C5-C4	-6.88	1.33	1.38
22	BA	2406	A	C5-C4	-6.88	1.33	1.38
1	AA	1429	A	C5-C4	-6.88	1.33	1.38
22	BA	1637	A	C5-C4	-6.88	1.33	1.38
22	BA	2792	A	C5-C4	-6.88	1.33	1.38
22	BA	294	A	C5-C4	-6.87	1.33	1.38
22	BA	1143	A	C5-C4	-6.87	1.33	1.38
22	BA	21	A	C5-C4	-6.87	1.33	1.38
22	BA	447	A	C5-C4	-6.87	1.33	1.38
22	BA	1147	A	C8-N7	6.87	1.36	1.31
22	BA	1819	A	C5-C4	-6.87	1.33	1.38
22	BA	1937	A	C8-N7	6.87	1.36	1.31
1	AA	784	A	C5-C4	-6.87	1.33	1.38
22	BA	167	A	C8-N7	6.87	1.36	1.31
22	BA	1700	A	C5-C4	-6.87	1.33	1.38
1	AA	533	A	C8-N7	6.87	1.36	1.31
22	BA	49	A	C5-C4	-6.87	1.33	1.38
22	BA	2266	A	C8-N7	6.86	1.36	1.31
22	BA	861	A	C5-C4	-6.86	1.33	1.38
22	BA	2268	A	C5-C4	-6.86	1.33	1.38
1	AA	397	A	C8-N7	6.86	1.36	1.31
22	BA	2378	A	C5-C4	-6.86	1.33	1.38
22	BA	1745	A	C8-N7	6.86	1.36	1.31
1	AA	583	A	C5-C4	-6.86	1.33	1.38
1	AA	743	A	C8-N7	6.86	1.36	1.31
1	AA	819	A	C8-N7	6.86	1.36	1.31
22	BA	6	A	C8-N7	6.86	1.36	1.31
22	BA	218	A	C5-C4	-6.86	1.33	1.38
22	BA	1744	A	C8-N7	6.86	1.36	1.31
1	AA	1319	A	C8-N7	6.85	1.36	1.31
1	AA	865	A	C8-N7	6.85	1.36	1.31
1	AA	915	A	C5-C4	-6.85	1.33	1.38
22	BA	1147	A	C5-C4	-6.85	1.33	1.38
22	BA	1678	A	C5-C4	-6.85	1.33	1.38
22	BA	514	A	C5-C4	-6.85	1.33	1.38
22	BA	2766	A	C5-C4	-6.85	1.33	1.38
1	AA	816	A	C5-C4	-6.85	1.33	1.38
22	BA	979	A	C5-C4	-6.85	1.33	1.38
22	BA	1912	A	C5-C4	-6.85	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	371	A	C8-N7	6.85	1.36	1.31
22	BA	504	A	C5-C4	-6.85	1.33	1.38
22	BA	231	A	C8-N7	6.84	1.36	1.31
22	BA	802	A	C5-C4	-6.84	1.33	1.38
22	BA	2740	A	C8-N7	6.84	1.36	1.31
1	AA	807	A	C8-N7	6.84	1.36	1.31
22	BA	1302	A	C5-C4	-6.84	1.33	1.38
1	AA	574	A	C8-N7	6.84	1.36	1.31
22	BA	2829	A	C5-C4	-6.84	1.33	1.38
23	BB	99	A	C5-C4	-6.84	1.33	1.38
53	B5	24	PRO	N-CA	-6.84	1.35	1.47
1	AA	781	A	C8-N7	6.84	1.36	1.31
22	BA	1165	A	C5-C4	-6.84	1.33	1.38
22	BA	2062	A	C8-N7	6.84	1.36	1.31
22	BA	2734	A	C8-N7	6.84	1.36	1.31
1	AA	1081	A	C8-N7	6.83	1.36	1.31
22	BA	1853	A	C5-C4	-6.83	1.33	1.38
1	AA	790	A	C8-N7	6.83	1.36	1.31
22	BA	529	A	C5-C4	-6.83	1.33	1.38
22	BA	602	A	C8-N7	6.83	1.36	1.31
22	BA	705	A	C5-C4	-6.83	1.33	1.38
22	BA	1395	A	C5-C4	-6.83	1.33	1.38
22	BA	1247	A	C8-N7	6.83	1.36	1.31
22	BA	2590	A	C5-C4	-6.83	1.33	1.38
22	BA	1008	A	C5-C4	-6.83	1.33	1.38
22	BA	2886	A	C5-C4	-6.83	1.33	1.38
1	AA	715	A	C8-N7	6.83	1.36	1.31
22	BA	2814	A	C8-N7	6.83	1.36	1.31
1	AA	1428	A	C8-N7	6.83	1.36	1.31
22	BA	131	A	C5-C4	-6.83	1.33	1.38
22	BA	2439	A	C5-C4	-6.83	1.33	1.38
22	BA	95	A	C8-N7	6.82	1.36	1.31
23	BB	57	A	C8-N7	6.82	1.36	1.31
22	BA	83	A	C8-N7	6.82	1.36	1.31
22	BA	265	A	C5-C4	-6.82	1.33	1.38
22	BA	1366	A	C5-C4	-6.82	1.33	1.38
22	BA	1969	A	C5-C4	-6.82	1.33	1.38
22	BA	1927	A	C5-C4	-6.82	1.33	1.38
1	AA	1394	A	C5-C4	-6.82	1.33	1.38
22	BA	1551	A	C8-N7	6.82	1.36	1.31
55	B8	20	U	C2-N3	6.82	1.42	1.37
22	BA	503	A	C8-N7	6.82	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	845	A	C5-C4	-6.82	1.33	1.38
22	BA	2388	A	N3-C4	6.82	1.39	1.34
1	AA	1429	A	C8-N7	6.81	1.36	1.31
22	BA	2887	A	C5-C4	-6.81	1.33	1.38
1	AA	892	A	C8-N7	6.81	1.36	1.31
22	BA	677	A	C5-C4	-6.81	1.33	1.38
55	B8	6	A	C8-N7	6.81	1.36	1.31
22	BA	718	A	C5-C4	-6.81	1.33	1.38
22	BA	2386	A	C5-C4	-6.81	1.33	1.38
1	AA	1081	A	C5-C4	-6.81	1.33	1.38
22	BA	483	A	C5-C4	-6.80	1.33	1.38
22	BA	1169	A	C5-C4	-6.80	1.33	1.38
22	BA	1269	A	C5-C4	-6.80	1.33	1.38
22	BA	2705	A	C5-C4	-6.80	1.33	1.38
22	BA	2883	A	C5-C4	-6.80	1.33	1.38
22	BA	2173	A	N3-C4	6.80	1.39	1.34
22	BA	181	A	C5-C4	-6.80	1.33	1.38
22	BA	675	A	C5-C4	-6.80	1.33	1.38
22	BA	1204	A	C5-C4	-6.80	1.33	1.38
22	BA	1598	A	C5-C4	-6.80	1.33	1.38
22	BA	191	A	C5-C4	-6.80	1.33	1.38
22	BA	1791	A	C5-C4	-6.80	1.33	1.38
22	BA	1848	A	C5-C4	-6.80	1.33	1.38
22	BA	1876	A	C5-C4	-6.80	1.33	1.38
22	BA	2273	A	C5-C4	-6.80	1.33	1.38
22	BA	479	A	C8-N7	6.79	1.36	1.31
22	BA	2205	A	C5-C4	-6.79	1.33	1.38
1	AA	246	A	C5-C4	-6.79	1.33	1.38
22	BA	800	A	C5-C4	-6.79	1.33	1.38
22	BA	983	A	C5-C4	-6.79	1.33	1.38
22	BA	71	A	C5-C4	-6.79	1.33	1.38
22	BA	2868	A	C5-C4	-6.79	1.33	1.38
1	AA	309	A	C5-C4	-6.79	1.33	1.38
22	BA	722	A	C8-N7	6.79	1.36	1.31
22	BA	432	A	C8-N7	6.79	1.36	1.31
22	BA	753	A	C5-C4	-6.79	1.33	1.38
22	BA	1254	A	C5-C4	-6.79	1.33	1.38
22	BA	2270	A	C5-C4	-6.79	1.33	1.38
55	B8	69	A	C8-N7	6.79	1.36	1.31
22	BA	1194	A	C8-N7	6.79	1.36	1.31
22	BA	2288	A	C8-N7	6.79	1.36	1.31
1	AA	1499	A	C5-C4	-6.78	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	781	A	C8-N7	6.78	1.36	1.31
22	BA	1754	A	C5-C4	-6.78	1.34	1.38
1	AA	327	A	C5-C4	-6.78	1.34	1.38
22	BA	103	A	C5-C4	-6.78	1.34	1.38
23	BB	39	A	C5-C4	-6.78	1.34	1.38
1	AA	1163	A	C5-C4	-6.78	1.34	1.38
22	BA	1246	A	C5-C4	-6.78	1.34	1.38
22	BA	2426	A	C5-C4	-6.78	1.34	1.38
1	AA	816	A	C8-N7	6.77	1.36	1.31
22	BA	244	A	C5-C4	-6.77	1.34	1.38
22	BA	1548	A	C8-N7	6.77	1.36	1.31
22	BA	988	A	C5-C4	-6.77	1.34	1.38
22	BA	173	A	C5-C4	-6.77	1.34	1.38
1	AA	459	A	N3-C4	6.77	1.39	1.34
1	AA	780	A	C8-N7	6.76	1.36	1.31
22	BA	2478	A	C8-N7	6.76	1.36	1.31
22	BA	2882	A	C5-C4	-6.76	1.34	1.38
22	BA	2369	A	C5-C4	-6.76	1.34	1.38
1	AA	596	A	C5-C4	-6.76	1.34	1.38
1	AA	814	A	C5-C4	-6.76	1.34	1.38
22	BA	2757	A	C8-N7	6.76	1.36	1.31
1	AA	715	A	C5-C4	-6.76	1.34	1.38
22	BA	2247	A	C5-C4	-6.76	1.34	1.38
22	BA	173	A	C8-N7	6.76	1.36	1.31
22	BA	345	A	C8-N7	6.76	1.36	1.31
22	BA	863	A	C5-C4	-6.76	1.34	1.38
22	BA	1689	A	C5-C4	-6.76	1.34	1.38
22	BA	1890	A	C8-N7	6.75	1.36	1.31
22	BA	706	A	C5-C4	-6.75	1.34	1.38
1	AA	160	A	C5-C4	-6.75	1.34	1.38
22	BA	689	A	C5-C4	-6.75	1.34	1.38
1	AA	238	A	C5-C4	-6.75	1.34	1.38
22	BA	1387	A	C8-N7	6.74	1.36	1.31
22	BA	91	A	C8-N7	6.74	1.36	1.31
22	BA	1913	A	C5-C4	-6.74	1.34	1.38
1	AA	572	A	C5-C4	-6.74	1.34	1.38
22	BA	1453	A	C5-C4	-6.74	1.34	1.38
22	BA	2826	A	C5-C4	-6.74	1.34	1.38
22	BA	1439	A	C5-C4	-6.74	1.34	1.38
1	AA	329	A	C8-N7	6.73	1.36	1.31
1	AA	1433	A	C8-N7	6.73	1.36	1.31
22	BA	6	A	C5-C4	-6.73	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2198	A	C5-C4	-6.73	1.34	1.38
22	BA	2205	A	C8-N7	6.73	1.36	1.31
22	BA	2820	A	C5-C4	-6.73	1.34	1.38
1	AA	120	A	C5-C4	-6.73	1.34	1.38
22	BA	127	A	C5-C4	-6.73	1.34	1.38
22	BA	182	A	C8-N7	6.73	1.36	1.31
22	BA	2333	A	C5-C4	-6.73	1.34	1.38
1	AA	236	A	C5-C4	-6.73	1.34	1.38
1	AA	663	A	C5-C4	-6.73	1.34	1.38
1	AA	1410	A	C5-C4	-6.73	1.34	1.38
22	BA	429	A	C5-C4	-6.73	1.34	1.38
1	AA	907	A	C8-N7	6.72	1.36	1.31
22	BA	979	A	C8-N7	6.72	1.36	1.31
22	BA	2015	A	C5-C4	-6.72	1.34	1.38
22	BA	430	A	C8-N7	6.72	1.36	1.31
1	AA	1431	A	C5-C4	-6.72	1.34	1.38
10	AJ	39	PRO	N-CA	-6.72	1.35	1.47
22	BA	2327	A	N3-C4	6.72	1.38	1.34
22	BA	2298	A	C8-N7	6.72	1.36	1.31
22	BA	2434	A	C5-C4	-6.72	1.34	1.38
22	BA	1286	A	C8-N7	6.71	1.36	1.31
22	BA	265	A	C8-N7	6.71	1.36	1.31
22	BA	1890	A	C5-C4	-6.71	1.34	1.38
22	BA	2241	A	C8-N7	6.71	1.36	1.31
22	BA	804	A	C8-N7	6.71	1.36	1.31
1	AA	802	A	C8-N7	6.71	1.36	1.31
22	BA	2154	A	N3-C4	6.71	1.38	1.34
55	B8	6	A	C5-C4	-6.71	1.34	1.38
1	AA	151	A	C5-C4	-6.71	1.34	1.38
22	BA	310	A	C5-C4	-6.71	1.34	1.38
22	BA	1553	A	C5-C4	-6.71	1.34	1.38
22	BA	2665	A	C8-N7	6.71	1.36	1.31
22	BA	602	A	C5-C4	-6.70	1.34	1.38
22	BA	1189	A	N3-C4	6.70	1.38	1.34
22	BA	528	A	C5-C4	-6.70	1.34	1.38
1	AA	8	A	C5-C4	-6.70	1.34	1.38
22	BA	480	A	C5-C4	-6.70	1.34	1.38
22	BA	782	A	N3-C4	6.70	1.38	1.34
22	BA	2450	A	C8-N7	6.70	1.36	1.31
22	BA	508	A	C5-C4	-6.70	1.34	1.38
22	BA	2376	A	C8-N7	6.70	1.36	1.31
22	BA	1165	A	C8-N7	6.70	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	53	A	C5-C4	-6.69	1.34	1.38
22	BA	1134	A	C8-N7	6.69	1.36	1.31
22	BA	1981	A	C5-C4	-6.69	1.34	1.38
22	BA	2411	A	C5-C4	-6.69	1.34	1.38
22	BA	1551	A	C5-C4	-6.69	1.34	1.38
22	BA	1677	A	C5-C4	-6.69	1.34	1.38
22	BA	2314	A	C5-C4	-6.69	1.34	1.38
22	BA	2810	A	C8-N7	6.69	1.36	1.31
22	BA	1393	A	C5-C4	-6.69	1.34	1.38
22	BA	975	A	C8-N7	6.69	1.36	1.31
22	BA	2799	A	C8-N7	6.69	1.36	1.31
22	BA	1810	A	C5-C4	-6.68	1.34	1.38
1	AA	498	A	C5-C4	-6.68	1.34	1.38
1	AA	845	A	N3-C4	6.68	1.38	1.34
22	BA	1566	A	C8-N7	6.68	1.36	1.31
22	BA	1953	A	C5-C4	-6.68	1.34	1.38
22	BA	2031	A	C8-N7	6.68	1.36	1.31
22	BA	2241	A	C5-C4	-6.68	1.34	1.38
22	BA	2328	A	C5-C4	-6.68	1.34	1.38
22	BA	71	A	C8-N7	6.68	1.36	1.31
22	BA	1477	A	C5-C4	-6.68	1.34	1.38
22	BA	1987	A	C8-N7	6.68	1.36	1.31
1	AA	353	A	C5-C4	-6.68	1.34	1.38
22	BA	1640	A	C8-N7	6.68	1.36	1.31
22	BA	1214	A	C5-C4	-6.68	1.34	1.38
22	BA	2158	A	N3-C4	6.68	1.38	1.34
22	BA	1593	A	C5-C4	-6.67	1.34	1.38
22	BA	1745	A	C5-C4	-6.67	1.34	1.38
22	BA	2322	A	C8-N7	6.67	1.36	1.31
22	BA	332	A	C8-N7	6.67	1.36	1.31
22	BA	756	A	C5-C4	-6.67	1.34	1.38
22	BA	1630	A	C5-C4	-6.67	1.34	1.38
22	BA	2547	A	C5-C4	-6.67	1.34	1.38
1	AA	1333	A	N3-C4	6.67	1.38	1.34
22	BA	1545	A	C5-C4	-6.67	1.34	1.38
22	BA	2468	A	C8-N7	6.67	1.36	1.31
1	AA	371	A	C5-C4	-6.66	1.34	1.38
22	BA	95	A	C5-C4	-6.66	1.34	1.38
22	BA	227	A	C8-N7	6.66	1.36	1.31
22	BA	1365	A	C5-C4	-6.66	1.34	1.38
22	BA	141	G	C6-N1	-6.66	1.34	1.39
1	AA	26	A	C5-C4	-6.66	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1465	A	C8-N7	6.66	1.36	1.31
22	BA	422	A	C8-N7	6.66	1.36	1.31
22	BA	2566	A	C5-C4	-6.66	1.34	1.38
22	BA	2887	A	C8-N7	6.66	1.36	1.31
1	AA	675	A	C5-C4	-6.65	1.34	1.38
1	AA	1201	A	C5-C4	-6.65	1.34	1.38
1	AA	1229	A	C5-C4	-6.65	1.34	1.38
22	BA	590	A	C5-C4	-6.65	1.34	1.38
22	BA	2430	A	C5-C4	-6.65	1.34	1.38
22	BA	2665	A	C5-C4	-6.65	1.34	1.38
1	AA	320	A	C5-C4	-6.65	1.34	1.38
22	BA	103	A	C8-N7	6.65	1.36	1.31
1	AA	298	A	C5-C4	-6.65	1.34	1.38
1	AA	767	A	C8-N7	6.65	1.36	1.31
1	AA	1430	A	C8-N7	6.65	1.36	1.31
22	BA	1089	A	N3-C4	6.65	1.38	1.34
1	AA	1499	A	C8-N7	6.65	1.36	1.31
1	AA	768	A	C8-N7	6.64	1.36	1.31
22	BA	1773	A	C5-C4	-6.64	1.34	1.38
1	AA	914	A	C5-C4	-6.64	1.34	1.38
1	AA	77	A	N3-C4	6.64	1.38	1.34
1	AA	288	A	C5-C4	-6.64	1.34	1.38
1	AA	1239	A	C5-C4	-6.64	1.34	1.38
22	BA	756	A	C8-N7	6.64	1.36	1.31
22	BA	2298	A	C5-C4	-6.64	1.34	1.38
22	BA	1336	A	C5-C4	-6.64	1.34	1.38
55	B8	38	A	C5-C4	-6.64	1.34	1.38
22	BA	1090	A	N3-C4	6.64	1.38	1.34
22	BA	1504	A	C5-C4	-6.64	1.34	1.38
22	BA	2060	A	C8-N7	6.64	1.36	1.31
22	BA	104	A	C5-C4	-6.63	1.34	1.38
22	BA	251	A	N7-C5	-6.63	1.35	1.39
22	BA	1757	A	C5-C4	-6.63	1.34	1.38
22	BA	2778	A	C5-C4	-6.63	1.34	1.38
22	BA	1439	A	C8-N7	6.63	1.36	1.31
22	BA	1853	A	C8-N7	6.63	1.36	1.31
23	BB	108	A	C5-C4	-6.63	1.34	1.38
1	AA	1101	A	C5-C4	-6.63	1.34	1.38
1	AA	1332	A	C5-C4	-6.63	1.34	1.38
22	BA	149	A	C5-C4	-6.63	1.34	1.38
22	BA	155	A	C5-C4	-6.63	1.34	1.38
22	BA	909	A	C8-N7	6.63	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	920	A	C8-N7	6.63	1.36	1.31
22	BA	716	A	C5-C4	-6.63	1.34	1.38
22	BA	2873	A	C5-C4	-6.63	1.34	1.38
1	AA	1329	A	C5-C4	-6.62	1.34	1.38
22	BA	348	A	C5-C4	-6.62	1.34	1.38
22	BA	2461	A	C5-C4	-6.62	1.34	1.38
1	AA	694	A	C5-C4	-6.62	1.34	1.38
22	BA	217	A	C8-N7	6.62	1.36	1.31
22	BA	1327	A	C5-C4	-6.62	1.34	1.38
1	AA	1465	A	C5-C4	-6.62	1.34	1.38
22	BA	699	A	C8-N7	6.62	1.36	1.31
22	BA	927	A	C5-C4	-6.62	1.34	1.38
22	BA	1502	A	C5-C4	-6.62	1.34	1.38
22	BA	1528	A	N3-C4	6.62	1.38	1.34
22	BA	627	A	C8-N7	6.62	1.36	1.31
22	BA	1253	A	C8-N7	6.62	1.36	1.31
22	BA	1610	A	C5-C4	-6.62	1.34	1.38
22	BA	457	A	C5-C4	-6.61	1.34	1.38
22	BA	492	A	C5-C4	-6.61	1.34	1.38
22	BA	933	A	C8-N7	6.61	1.36	1.31
22	BA	1780	A	C8-N7	6.61	1.36	1.31
1	AA	609	A	C5-C4	-6.61	1.34	1.38
22	BA	1528	A	C5-C4	-6.61	1.34	1.38
1	AA	913	A	C5-C4	-6.61	1.34	1.38
22	BA	320	A	C8-N7	6.61	1.36	1.31
22	BA	1477	A	C8-N7	6.61	1.36	1.31
22	BA	1713	A	C5-C4	-6.61	1.34	1.38
1	AA	1151	A	N3-C4	6.60	1.38	1.34
22	BA	739	A	C5-C4	-6.60	1.34	1.38
22	BA	2340	A	C8-N7	6.60	1.36	1.31
22	BA	1496	A	C5-C4	-6.60	1.34	1.38
22	BA	2274	A	C5-C4	-6.60	1.34	1.38
22	BA	2632	A	C8-N7	6.60	1.36	1.31
22	BA	2748	A	C5-C4	-6.60	1.34	1.38
22	BA	2799	A	C2-N3	6.60	1.39	1.33
22	BA	1275	A	C5-C4	-6.60	1.34	1.38
22	BA	2284	A	C5-C4	-6.60	1.34	1.38
22	BA	2706	A	C5-C4	-6.60	1.34	1.38
1	AA	696	A	C8-N7	6.59	1.36	1.31
22	BA	1634	A	C8-N7	6.59	1.36	1.31
22	BA	515	A	C5-C4	-6.59	1.34	1.38
22	BA	1307	A	C5-C4	-6.59	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2809	A	C8-N7	6.59	1.36	1.31
1	AA	55	A	C8-N7	6.59	1.36	1.31
1	AA	743	A	C5-C4	-6.59	1.34	1.38
23	BB	109	A	C5-C4	-6.59	1.34	1.38
1	AA	553	A	C5-C4	-6.59	1.34	1.38
22	BA	2860	A	C8-N7	6.59	1.36	1.31
1	AA	1000	A	N3-C4	6.59	1.38	1.34
1	AA	1036	A	N3-C4	6.59	1.38	1.34
22	BA	1701	A	C5-C4	-6.59	1.34	1.38
22	BA	526	A	C8-N7	6.58	1.36	1.31
22	BA	1679	A	C5-C4	-6.58	1.34	1.38
22	BA	2598	A	C5-C4	-6.58	1.34	1.38
22	BA	2741	A	C5-C4	-6.58	1.34	1.38
1	AA	228	A	C5-C4	-6.58	1.34	1.38
22	BA	1470	A	C8-N7	6.58	1.36	1.31
22	BA	1665	A	C5-C4	-6.58	1.34	1.38
22	BA	21	A	C8-N7	6.57	1.36	1.31
22	BA	2776	A	C5-C4	-6.57	1.34	1.38
22	BA	2829	A	C8-N7	6.57	1.36	1.31
22	BA	342	A	C5-C4	-6.57	1.34	1.38
22	BA	1433	A	C5-C4	-6.57	1.34	1.38
22	BA	1597	A	C5-C4	-6.57	1.34	1.38
22	BA	2147	A	N3-C4	6.57	1.38	1.34
55	B8	41	A	C8-N7	6.57	1.36	1.31
22	BA	1327	A	C8-N7	6.57	1.36	1.31
1	AA	33	A	C8-N7	6.57	1.36	1.31
1	AA	1441	A	N3-C4	6.57	1.38	1.34
22	BA	1616	A	C5-C4	-6.57	1.34	1.38
22	BA	2516	A	C5-C4	-6.57	1.34	1.38
22	BA	5	A	C5-C4	-6.57	1.34	1.38
22	BA	1427	A	C5-C4	-6.57	1.34	1.38
22	BA	1698	A	C8-N7	6.57	1.36	1.31
1	AA	716	A	C5-C4	-6.56	1.34	1.38
22	BA	1544	A	C5-C4	-6.56	1.34	1.38
22	BA	216	A	C5-C4	-6.56	1.34	1.38
22	BA	497	A	C5-C4	-6.56	1.34	1.38
22	BA	616	A	C8-N7	6.56	1.36	1.31
22	BA	1433	A	C8-N7	6.56	1.36	1.31
22	BA	1749	A	C5-C4	-6.56	1.34	1.38
22	BA	2094	A	N3-C4	6.56	1.38	1.34
23	BB	59	A	C2-N3	6.56	1.39	1.33
22	BA	800	A	C8-N7	6.56	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	844	A	C5-C4	-6.56	1.34	1.38
22	BA	936	A	C8-N7	6.56	1.36	1.31
23	BB	29	A	C5-C4	-6.56	1.34	1.38
1	AA	907	A	C5-C4	-6.56	1.34	1.38
22	BA	1321	A	C5-C4	-6.56	1.34	1.38
22	BA	2311	A	C5-C4	-6.56	1.34	1.38
22	BA	2227	A	C5-C4	-6.56	1.34	1.38
22	BA	2281	A	C8-N7	6.56	1.36	1.31
22	BA	167	A	C5-C4	-6.55	1.34	1.38
22	BA	844	A	C8-N7	6.55	1.36	1.31
1	AA	975	A	C5-C4	-6.55	1.34	1.38
22	BA	1073	A	N3-C4	6.55	1.38	1.34
22	BA	1253	A	C5-C4	-6.55	1.34	1.38
22	BA	2199	A	C5-C4	-6.55	1.34	1.38
22	BA	2810	A	C5-C4	-6.55	1.34	1.38
22	BA	2639	A	C8-N7	6.55	1.36	1.31
22	BA	42	A	C5-C4	-6.55	1.34	1.38
22	BA	1552	A	C8-N7	6.55	1.36	1.31
22	BA	1596	A	C5-C4	-6.55	1.34	1.38
22	BA	2212	A	C5-C4	-6.55	1.34	1.38
22	BA	2682	A	C5-C4	-6.55	1.34	1.38
1	AA	498	A	C2-N3	6.55	1.39	1.33
1	AA	1428	A	C5-C4	-6.55	1.34	1.38
22	BA	1711	A	C8-N7	6.55	1.36	1.31
55	B8	14	A	C8-N7	6.55	1.36	1.31
22	BA	1641	A	C5-C4	-6.54	1.34	1.38
22	BA	1676	A	N3-C4	6.54	1.38	1.34
1	AA	33	A	C5-C4	-6.54	1.34	1.38
22	BA	761	A	N3-C4	6.54	1.38	1.34
22	BA	1301	A	C8-N7	6.54	1.36	1.31
22	BA	2317	A	C5-C4	-6.54	1.34	1.38
39	BR	52	PRO	N-CA	-6.54	1.36	1.47
22	BA	504	A	N3-C4	6.54	1.38	1.34
22	BA	2062	A	C5-C4	-6.54	1.34	1.38
22	BA	2856	A	C5-C4	-6.54	1.34	1.38
22	BA	262	A	N3-C4	6.54	1.38	1.34
22	BA	764	A	C8-N7	6.54	1.36	1.31
22	BA	981	A	C5-C4	-6.54	1.34	1.38
1	AA	116	A	C5-C4	-6.54	1.34	1.38
22	BA	118	A	C5-C4	-6.54	1.34	1.38
22	BA	2425	A	C5-C4	-6.54	1.34	1.38
1	AA	349	A	C5-C4	-6.53	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	563	A	C8-N7	6.53	1.36	1.31
22	BA	2764	A	C5-C4	-6.53	1.34	1.38
1	AA	1413	A	C5-C4	-6.53	1.34	1.38
22	BA	2142	A	N3-C4	6.53	1.38	1.34
22	BA	526	A	C5-C4	-6.53	1.34	1.38
22	BA	1126	A	C5-C4	-6.53	1.34	1.38
22	BA	1301	A	C5-C4	-6.53	1.34	1.38
1	AA	608	A	C5-C4	-6.53	1.34	1.38
1	AA	759	A	C5-C4	-6.53	1.34	1.38
1	AA	32	A	C5-C4	-6.53	1.34	1.38
1	AA	60	A	C5-C4	-6.53	1.34	1.38
1	AA	315	A	C5-C4	-6.53	1.34	1.38
1	AA	1398	A	C5-C4	-6.53	1.34	1.38
22	BA	402	A	C5-C4	-6.53	1.34	1.38
22	BA	1746	A	C8-N7	6.53	1.36	1.31
22	BA	2741	A	C8-N7	6.53	1.36	1.31
22	BA	2749	A	N3-C4	6.53	1.38	1.34
1	AA	1261	A	N3-C4	6.52	1.38	1.34
22	BA	14	A	C5-C4	-6.52	1.34	1.38
22	BA	1032	A	C5-C4	-6.52	1.34	1.38
22	BA	1086	A	C5-C4	-6.52	1.34	1.38
22	BA	1373	A	C8-N7	6.52	1.36	1.31
1	AA	411	A	N3-C4	6.52	1.38	1.34
55	B8	73	A	C8-N7	6.52	1.36	1.31
22	BA	1111	A	C5-C4	-6.52	1.34	1.38
22	BA	1265	A	C8-N7	6.52	1.36	1.31
22	BA	1284	A	C8-N7	6.52	1.36	1.31
22	BA	2765	A	C5-C4	-6.52	1.34	1.38
22	BA	1754	A	C8-N7	6.52	1.36	1.31
22	BA	2037	A	C5-C4	-6.52	1.34	1.38
22	BA	845	A	N3-C4	6.51	1.38	1.34
22	BA	1336	A	C8-N7	6.51	1.36	1.31
22	BA	2031	A	N3-C4	6.51	1.38	1.34
1	AA	1163	A	N3-C4	6.51	1.38	1.34
1	AA	1483	A	C5-C4	-6.51	1.34	1.38
22	BA	1014	A	C5-C4	-6.51	1.34	1.38
22	BA	1237	A	C8-N7	6.51	1.36	1.31
22	BA	2346	A	C5-C4	-6.51	1.34	1.38
1	AA	1447	A	C5-C4	-6.51	1.34	1.38
22	BA	332	A	C5-C4	-6.51	1.34	1.38
22	BA	981	A	C8-N7	6.51	1.36	1.31
22	BA	2117	A	N3-C4	6.51	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2432	A	C5-C4	-6.51	1.34	1.38
22	BA	2726	A	C5-C4	-6.51	1.34	1.38
22	BA	63	A	C5-C4	-6.50	1.34	1.38
22	BA	783	A	C5-C4	-6.50	1.34	1.38
22	BA	310	A	C8-N7	6.50	1.36	1.31
22	BA	1001	A	C5-C4	-6.50	1.34	1.38
22	BA	1276	A	C5-C4	-6.50	1.34	1.38
22	BA	2434	A	C8-N7	6.50	1.36	1.31
1	AA	681	A	C5-C4	-6.50	1.34	1.38
1	AA	909	A	C5-C4	-6.50	1.34	1.38
1	AA	1196	A	C5-C4	-6.50	1.34	1.38
22	BA	152	A	C8-N7	6.50	1.36	1.31
22	BA	1274	A	C5-C4	-6.50	1.34	1.38
22	BA	1900	A	C8-N7	6.50	1.36	1.31
22	BA	1901	A	C8-N7	6.50	1.36	1.31
1	AA	878	A	C5-C4	-6.50	1.34	1.38
1	AA	1377	A	C5-C4	-6.50	1.34	1.38
22	BA	423	A	C5-C4	-6.50	1.34	1.38
22	BA	2163	A	N3-C4	6.50	1.38	1.34
22	BA	2134	A	N3-C4	6.50	1.38	1.34
1	AA	718	A	C5-C4	-6.49	1.34	1.38
22	BA	64	A	C8-N7	6.49	1.36	1.31
22	BA	466	A	C5-C4	-6.49	1.34	1.38
22	BA	655	A	C5-C4	-6.49	1.34	1.38
22	BA	1679	A	C8-N7	6.49	1.36	1.31
22	BA	2333	A	C8-N7	6.49	1.36	1.31
22	BA	222	A	C8-N7	6.49	1.36	1.31
22	BA	347	A	C5-C4	-6.49	1.34	1.38
22	BA	2560	A	C5-C4	-6.49	1.34	1.38
22	BA	160	A	C5-C4	-6.49	1.34	1.38
22	BA	1803	A	N3-C4	6.49	1.38	1.34
22	BA	2639	A	C5-C4	-6.49	1.34	1.38
22	BA	1134	A	C5-C4	-6.49	1.34	1.38
23	BB	104	A	C8-N7	6.49	1.36	1.31
1	AA	716	A	C8-N7	6.48	1.36	1.31
1	AA	794	A	C5-C4	-6.48	1.34	1.38
23	BB	59	A	C8-N7	6.48	1.36	1.31
22	BA	505	A	C5-C4	-6.48	1.34	1.38
22	BA	1634	A	C5-C4	-6.48	1.34	1.38
1	AA	2	A	C5-C4	-6.48	1.34	1.38
1	AA	243	A	C5-C4	-6.48	1.34	1.38
22	BA	918	A	C5-C4	-6.48	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2270	A	C8-N7	6.48	1.36	1.31
1	AA	706	A	N3-C4	6.48	1.38	1.34
22	BA	833	A	C5-C4	-6.48	1.34	1.38
22	BA	945	A	C5-C4	-6.48	1.34	1.38
23	BB	73	A	C8-N7	6.48	1.36	1.31
1	AA	918	A	C5-C4	-6.48	1.34	1.38
22	BA	241	A	C5-C4	-6.48	1.34	1.38
22	BA	1189	A	C5-C4	-6.47	1.34	1.38
1	AA	53	A	C5-C4	-6.47	1.34	1.38
22	BA	2051	A	C5-C4	-6.47	1.34	1.38
22	BA	2336	A	C5-C4	-6.47	1.34	1.38
22	BA	89	A	C5-C4	-6.47	1.34	1.38
22	BA	1040	A	C5-C4	-6.47	1.34	1.38
1	AA	80	A	N3-C4	6.47	1.38	1.34
22	BA	927	A	C8-N7	6.47	1.36	1.31
22	BA	1378	A	C8-N7	6.47	1.36	1.31
22	BA	2476	A	C5-C4	-6.47	1.34	1.38
22	BA	637	A	C5-C4	-6.47	1.34	1.38
22	BA	2088	A	C5-C4	-6.47	1.34	1.38
22	BA	2733	A	C5-C4	-6.47	1.34	1.38
1	AA	412	A	N3-C4	6.46	1.38	1.34
22	BA	1156	A	N3-C4	6.46	1.38	1.34
55	B8	66	A	C8-N7	6.46	1.36	1.31
1	AA	1	A	N3-C4	6.46	1.38	1.34
1	AA	3	A	C5-C4	-6.46	1.34	1.38
1	AA	1434	A	C5-C4	-6.46	1.34	1.38
22	BA	1272	A	C8-N7	6.46	1.36	1.31
22	BA	1503	A	C5-C4	-6.46	1.34	1.38
22	BA	401	A	C5-C4	-6.46	1.34	1.38
22	BA	478	A	C8-N7	6.46	1.36	1.31
22	BA	1783	A	C5-C4	-6.46	1.34	1.38
22	BA	2031	A	C5-C4	-6.46	1.34	1.38
22	BA	2184	A	N3-C4	6.46	1.38	1.34
1	AA	197	A	C5-C4	-6.46	1.34	1.38
22	BA	1701	A	C8-N7	6.46	1.36	1.31
22	BA	1801	A	C8-N7	6.46	1.36	1.31
1	AA	10	A	C5-C4	-6.45	1.34	1.38
1	AA	523	A	C5-C4	-6.45	1.34	1.38
22	BA	513	A	N7-C5	-6.45	1.35	1.39
22	BA	2837	A	C5-C4	-6.45	1.34	1.38
1	AA	499	A	C5-C4	-6.45	1.34	1.38
22	BA	943	A	C5-C4	-6.45	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1009	A	C5-C4	-6.45	1.34	1.38
22	BA	2565	A	C5-C4	-6.45	1.34	1.38
22	BA	960	A	N3-C4	6.45	1.38	1.34
1	AA	802	A	C5-C4	-6.45	1.34	1.38
1	AA	914	A	C8-N7	6.45	1.36	1.31
22	BA	346	A	C5-C4	-6.45	1.34	1.38
22	BA	633	A	C8-N7	6.45	1.36	1.31
22	BA	706	A	C8-N7	6.45	1.36	1.31
22	BA	804	A	C5-C4	-6.45	1.34	1.38
22	BA	1522	A	C5-C4	-6.45	1.34	1.38
22	BA	1784	A	C5-C4	-6.45	1.34	1.38
22	BA	1872	A	C8-N7	6.45	1.36	1.31
22	BA	1877	A	C5-C4	-6.45	1.34	1.38
22	BA	2154	A	C5-C4	-6.45	1.34	1.38
22	BA	1532	A	C5-C4	-6.44	1.34	1.38
1	AA	356	A	C5-C4	-6.44	1.34	1.38
22	BA	502	A	C5-C4	-6.44	1.34	1.38
22	BA	782	A	C5-C4	-6.44	1.34	1.38
22	BA	1111	A	N3-C4	6.44	1.38	1.34
22	BA	1431	A	C5-C4	-6.44	1.34	1.38
22	BA	1626	A	C8-N7	6.44	1.36	1.31
22	BA	1509	A	C5-C4	-6.44	1.34	1.38
1	AA	1431	A	C8-N7	6.44	1.36	1.31
22	BA	508	A	N3-C4	6.44	1.38	1.34
1	AA	51	A	C5-C4	-6.43	1.34	1.38
1	AA	602	A	C5-C4	-6.43	1.34	1.38
22	BA	1937	A	C5-C4	-6.43	1.34	1.38
22	BA	2381	A	C8-N7	6.43	1.36	1.31
1	AA	161	A	C5-C4	-6.43	1.34	1.38
1	AA	777	A	C5-C4	-6.43	1.34	1.38
22	BA	74	A	C5-C4	-6.43	1.34	1.38
22	BA	2412	A	C5-C4	-6.43	1.34	1.38
23	BB	52	A	C5-C4	-6.43	1.34	1.38
22	BA	1932	A	C8-N7	6.43	1.36	1.31
1	AA	55	A	C5-C4	-6.43	1.34	1.38
23	BB	78	A	C8-N7	6.43	1.36	1.31
22	BA	866	A	C8-N7	6.43	1.36	1.31
22	BA	1054	A	N3-C4	6.43	1.38	1.34
22	BA	2377	A	C8-N7	6.43	1.36	1.31
1	AA	574	A	C5-C4	-6.42	1.34	1.38
22	BA	38	A	C5-C4	-6.42	1.34	1.38
22	BA	1230	A	C8-N7	6.42	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2322	A	C5-C4	-6.42	1.34	1.38
55	B8	26	A	C5-C4	-6.42	1.34	1.38
55	B8	58	A	C5-C4	-6.42	1.34	1.38
1	AA	600	A	C5-C4	-6.42	1.34	1.38
22	BA	522	A	C5-C4	-6.42	1.34	1.38
22	BA	1632	A	C8-N7	6.42	1.36	1.31
1	AA	1289	A	C5-C4	-6.42	1.34	1.38
22	BA	1614	A	C8-N7	6.42	1.36	1.31
22	BA	2183	A	N3-C4	6.42	1.38	1.34
1	AA	1339	A	C8-N7	6.42	1.36	1.31
22	BA	1854	A	C5-C4	-6.42	1.34	1.38
1	AA	1318	A	C5-C4	-6.42	1.34	1.38
22	BA	2682	A	C8-N7	6.42	1.36	1.31
23	BB	34	A	C5-C4	-6.42	1.34	1.38
1	AA	1275	A	C5-C4	-6.42	1.34	1.38
1	AA	1507	A	C5-C4	-6.42	1.34	1.38
22	BA	960	A	N7-C5	-6.41	1.35	1.39
22	BA	2757	A	N3-C4	6.41	1.38	1.34
1	AA	1299	A	C5-C4	-6.41	1.34	1.38
1	AA	364	A	C5-C4	-6.41	1.34	1.38
1	AA	468	A	N3-C4	6.41	1.38	1.34
1	AA	1492	A	C5-C4	-6.41	1.34	1.38
22	BA	2327	A	C5-C4	-6.41	1.34	1.38
1	AA	1513	A	C5-C4	-6.41	1.34	1.38
22	BA	477	A	C5-C4	-6.41	1.34	1.38
22	BA	1048	A	N3-C4	6.41	1.38	1.34
22	BA	1899	A	C5-C4	-6.41	1.34	1.38
1	AA	665	A	C5-C4	-6.41	1.34	1.38
1	AA	510	A	C5-C4	-6.40	1.34	1.38
1	AA	712	A	C5-C4	-6.40	1.34	1.38
22	BA	83	A	C5-C4	-6.40	1.34	1.38
22	BA	13	A	C8-N7	6.40	1.36	1.31
22	BA	216	A	C8-N7	6.40	1.36	1.31
23	BB	119	A	N3-C4	6.40	1.38	1.34
22	BA	715	A	C5-C4	-6.40	1.34	1.38
1	AA	502	A	C5-C4	-6.39	1.34	1.38
1	AA	1257	A	N3-C4	6.39	1.38	1.34
22	BA	928	A	C5-C4	-6.39	1.34	1.38
22	BA	1572	A	C5-C4	-6.39	1.34	1.38
22	BA	2378	A	C8-N7	6.39	1.36	1.31
22	BA	829	A	C5-C4	-6.39	1.34	1.38
22	BA	1960	A	C8-N7	6.39	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2171	A	N3-C4	6.39	1.38	1.34
1	AA	172	A	C5-C4	-6.39	1.34	1.38
1	AA	181	A	C5-C4	-6.39	1.34	1.38
1	AA	676	A	C5-C4	-6.39	1.34	1.38
22	BA	1020	A	C5-C4	-6.39	1.34	1.38
22	BA	1084	A	N3-C4	6.39	1.38	1.34
22	BA	1698	A	C5-C4	-6.39	1.34	1.38
22	BA	2407	A	C5-C4	-6.39	1.34	1.38
1	AA	306	A	C5-C4	-6.39	1.34	1.38
1	AA	1201	A	N3-C4	6.38	1.38	1.34
22	BA	309	A	C8-N7	6.38	1.36	1.31
22	BA	449	A	C5-C4	-6.38	1.34	1.38
22	BA	2531	A	C5-C4	-6.38	1.34	1.38
22	BA	2776	A	C8-N7	6.38	1.36	1.31
1	AA	640	A	C5-C4	-6.38	1.34	1.38
22	BA	1579	A	C5-C4	-6.38	1.34	1.38
22	BA	1928	A	C5-C4	-6.38	1.34	1.38
1	AA	143	A	C5-C4	-6.38	1.34	1.38
22	BA	782	A	C8-N7	6.38	1.36	1.31
22	BA	1080	A	N3-C4	6.38	1.38	1.34
22	BA	1359	A	C8-N7	6.38	1.36	1.31
1	AA	1000	A	C5-C4	-6.38	1.34	1.38
22	BA	1609	A	C8-N7	6.38	1.36	1.31
22	BA	1783	A	N3-C4	6.38	1.38	1.34
1	AA	74	A	C5-C4	-6.38	1.34	1.38
1	AA	1408	A	C5-C4	-6.38	1.34	1.38
1	AA	59	A	C5-C4	-6.37	1.34	1.38
1	AA	78	A	N3-C4	6.37	1.38	1.34
1	AA	495	A	C5-C4	-6.37	1.34	1.38
1	AA	1256	A	C5-C4	-6.37	1.34	1.38
22	BA	1098	A	N3-C4	6.37	1.38	1.34
22	BA	2518	A	C8-N7	6.37	1.36	1.31
1	AA	935	A	C5-C4	-6.37	1.34	1.38
1	AA	1483	A	N3-C4	6.37	1.38	1.34
22	BA	1610	A	C8-N7	6.37	1.36	1.31
22	BA	152	A	C5-C4	-6.37	1.34	1.38
22	BA	2126	A	N3-C4	6.37	1.38	1.34
1	AA	1117	A	C5-C4	-6.37	1.34	1.38
22	BA	204	A	C8-N7	6.37	1.36	1.31
22	BA	311	A	C8-N7	6.37	1.36	1.31
1	AA	119	A	C5-C4	-6.37	1.34	1.38
22	BA	502	A	C8-N7	6.37	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1214	A	C8-N7	6.37	1.36	1.31
22	BA	2005	A	C5-C4	-6.37	1.34	1.38
23	BB	119	A	C5-C4	-6.37	1.34	1.38
1	AA	946	A	C5-C4	-6.37	1.34	1.38
22	BA	2662	A	C8-N7	6.37	1.36	1.31
22	BA	2711	A	N3-C4	6.37	1.38	1.34
1	AA	44	A	C5-C4	-6.36	1.34	1.38
22	BA	990	A	C5-C4	-6.36	1.34	1.38
22	BA	2169	A	N3-C4	6.36	1.38	1.34
22	BA	2711	A	C8-N7	6.36	1.36	1.31
22	BA	2900	A	C5-C4	-6.36	1.34	1.38
1	AA	781	A	C5-C4	-6.36	1.34	1.38
22	BA	654	A	C5-C4	-6.36	1.34	1.38
22	BA	1057	A	N3-C4	6.36	1.38	1.34
22	BA	1552	A	C5-C4	-6.36	1.34	1.38
22	BA	2411	A	C8-N7	6.36	1.36	1.31
22	BA	616	A	C5-C4	-6.36	1.34	1.38
1	AA	389	A	N3-C4	6.36	1.38	1.34
1	AA	456	A	C5-C4	-6.36	1.34	1.38
22	BA	1021	A	C5-C4	-6.36	1.34	1.38
1	AA	53	A	N3-C4	6.36	1.38	1.34
1	AA	321	A	C5-C4	-6.36	1.34	1.38
12	AL	45	PRO	N-CA	-6.36	1.36	1.47
22	BA	196	A	C8-N7	6.36	1.35	1.31
22	BA	272	A	C5-C4	-6.36	1.34	1.38
22	BA	2278	A	C5-C4	-6.36	1.34	1.38
23	BB	58	A	C5-C4	-6.36	1.34	1.38
23	BB	59	A	N3-C4	6.36	1.38	1.34
1	AA	109	A	C5-C4	-6.35	1.34	1.38
1	AA	533	A	N3-C4	6.35	1.38	1.34
1	AA	560	A	C5-C4	-6.35	1.34	1.38
22	BA	64	A	C5-C4	-6.35	1.34	1.38
22	BA	1096	A	N3-C4	6.35	1.38	1.34
22	BA	2335	A	N3-C4	6.35	1.38	1.34
22	BA	2614	A	C5-C4	-6.35	1.34	1.38
1	AA	344	A	C5-C4	-6.35	1.34	1.38
22	BA	1505	A	C5-C4	-6.35	1.34	1.38
22	BA	2850	A	C8-N7	6.35	1.35	1.31
22	BA	53	A	C8-N7	6.34	1.35	1.31
22	BA	497	A	C8-N7	6.34	1.35	1.31
22	BA	973	A	C5-C4	-6.34	1.34	1.38
22	BA	1095	A	N3-C4	6.34	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1418	A	C5-C4	-6.34	1.34	1.38
22	BA	1918	A	C5-C4	-6.34	1.34	1.38
22	BA	2297	A	C5-C4	-6.34	1.34	1.38
1	AA	383	A	N3-C4	6.34	1.38	1.34
22	BA	1916	A	C5-C4	-6.34	1.34	1.38
22	BA	2281	A	C5-C4	-6.34	1.34	1.38
22	BA	2813	A	C5-C4	-6.34	1.34	1.38
23	BB	101	A	C5-C4	-6.34	1.34	1.38
1	AA	130	A	C5-C4	-6.34	1.34	1.38
1	AA	373	A	N3-C4	6.34	1.38	1.34
1	AA	825	A	C5-C4	-6.34	1.34	1.38
1	AA	1157	A	N3-C4	6.34	1.38	1.34
1	AA	655	A	C5-C4	-6.34	1.34	1.38
22	BA	422	A	N3-C4	6.34	1.38	1.34
22	BA	899	A	C5-C4	-6.34	1.34	1.38
22	BA	1496	A	N3-C4	6.34	1.38	1.34
22	BA	1669	A	N3-C4	6.34	1.38	1.34
22	BA	182	A	C5-C4	-6.33	1.34	1.38
1	AA	906	A	C5-C4	-6.33	1.34	1.38
22	BA	374	A	C8-N7	6.33	1.35	1.31
22	BA	2560	A	C8-N7	6.33	1.35	1.31
55	B8	41	A	C5-C4	-6.33	1.34	1.38
1	AA	171	A	N3-C4	6.33	1.38	1.34
22	BA	101	A	C5-C4	-6.33	1.34	1.38
55	B8	51	A	C5-C4	-6.33	1.34	1.38
1	AA	1502	A	C5-C4	-6.33	1.34	1.38
1	AA	456	A	N3-C4	6.33	1.38	1.34
1	AA	1252	A	N3-C4	6.33	1.38	1.34
22	BA	412	A	C5-C4	-6.33	1.34	1.38
22	BA	2114	A	N3-C4	6.33	1.38	1.34
22	BA	282	A	C5-C4	-6.33	1.34	1.38
22	BA	256	A	C5-C4	-6.33	1.34	1.38
22	BA	783	A	N3-C4	6.33	1.38	1.34
22	BA	1127	A	C5-C4	-6.33	1.34	1.38
1	AA	937	A	C5-C4	-6.32	1.34	1.38
1	AA	573	A	C5-C4	-6.32	1.34	1.38
22	BA	1928	A	C8-N7	6.32	1.35	1.31
22	BA	2451	A	C5-C4	-6.32	1.34	1.38
1	AA	994	A	N3-C4	6.32	1.38	1.34
1	AA	1170	A	C8-N7	6.32	1.35	1.31
22	BA	13	A	C5-C4	-6.32	1.34	1.38
22	BA	478	A	C5-C4	-6.32	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2425	A	C8-N7	6.32	1.35	1.31
22	BA	482	A	C5-C4	-6.32	1.34	1.38
22	BA	1755	A	C8-N7	6.32	1.35	1.31
1	AA	408	A	N3-C4	6.32	1.38	1.34
1	AA	1157	A	C5-C4	-6.32	1.34	1.38
22	BA	1039	A	C5-C4	-6.32	1.34	1.38
22	BA	1260	A	C5-C4	-6.32	1.34	1.38
22	BA	199	A	C8-N7	6.31	1.35	1.31
22	BA	21	A	N3-C4	6.31	1.38	1.34
22	BA	627	A	C5-C4	-6.31	1.34	1.38
22	BA	1027	A	C8-N7	6.31	1.35	1.31
22	BA	226	A	C5-C4	-6.31	1.34	1.38
22	BA	928	A	C8-N7	6.31	1.35	1.31
22	BA	730	A	N3-C4	6.31	1.38	1.34
22	BA	1508	A	C5-C4	-6.31	1.34	1.38
22	BA	1690	A	C8-N7	6.31	1.35	1.31
22	BA	2266	A	C5-C4	-6.31	1.34	1.38
1	AA	129	A	C5-C4	-6.31	1.34	1.38
1	AA	807	A	C5-C4	-6.31	1.34	1.38
22	BA	279	A	C5-C4	-6.31	1.34	1.38
22	BA	1744	A	C5-C4	-6.31	1.34	1.38
22	BA	2750	A	C5-C4	-6.31	1.34	1.38
22	BA	2761	A	C5-C4	-6.31	1.34	1.38
1	AA	629	A	C5-C4	-6.31	1.34	1.38
1	AA	448	A	N3-C4	6.30	1.38	1.34
1	AA	794	A	C8-N7	6.30	1.35	1.31
1	AA	968	A	C5-C4	-6.30	1.34	1.38
22	BA	44	A	C5-C4	-6.30	1.34	1.38
22	BA	820	A	C5-C4	-6.30	1.34	1.38
1	AA	72	A	C5-C4	-6.30	1.34	1.38
1	AA	919	A	C5-C4	-6.30	1.34	1.38
22	BA	2706	A	C8-N7	6.30	1.35	1.31
1	AA	1145	A	N3-C4	6.30	1.38	1.34
22	BA	1571	A	N3-C4	6.30	1.38	1.34
1	AA	554	A	C5-C4	-6.30	1.34	1.38
22	BA	643	A	C8-N7	6.30	1.35	1.31
22	BA	1819	A	C8-N7	6.30	1.35	1.31
22	BA	127	A	C8-N7	6.30	1.35	1.31
22	BA	2119	A	N3-C4	6.30	1.38	1.34
1	AA	1275	A	N3-C4	6.30	1.38	1.34
22	BA	1308	A	N7-C5	-6.30	1.35	1.39
22	BA	1669	A	C8-N7	6.30	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2432	A	C8-N7	6.30	1.35	1.31
1	AA	1437	A	C5-C4	-6.29	1.34	1.38
22	BA	282	A	N3-C4	6.29	1.38	1.34
22	BA	1029	A	C5-C4	-6.29	1.34	1.38
1	AA	336	A	C5-C4	-6.29	1.34	1.38
22	BA	344	A	C5-C4	-6.29	1.34	1.38
22	BA	352	A	C5-C4	-6.29	1.34	1.38
22	BA	404	A	C5-C4	-6.29	1.34	1.38
22	BA	449	A	C8-N7	6.29	1.35	1.31
22	BA	590	A	C8-N7	6.29	1.35	1.31
22	BA	764	A	C5-C4	-6.29	1.34	1.38
22	BA	2327	A	C8-N7	6.29	1.35	1.31
1	AA	1219	A	N3-C4	6.29	1.38	1.34
22	BA	428	A	C8-N7	6.29	1.35	1.31
22	BA	2059	A	N3-C4	6.29	1.38	1.34
22	BA	2227	A	C8-N7	6.29	1.35	1.31
22	BA	2425	A	N3-C4	6.29	1.38	1.34
22	BA	149	A	C8-N7	6.29	1.35	1.31
22	BA	1054	A	C5-C4	-6.29	1.34	1.38
22	BA	1746	A	C5-C4	-6.29	1.34	1.38
1	AA	630	A	N3-C4	6.29	1.38	1.34
22	BA	278	A	N3-C4	6.29	1.38	1.34
1	AA	432	A	N3-C4	6.29	1.38	1.34
1	AA	1022	A	N3-C4	6.29	1.38	1.34
22	BA	1226	A	C5-C4	-6.29	1.34	1.38
1	AA	441	A	N3-C4	6.28	1.38	1.34
22	BA	507	A	C5-C4	-6.28	1.34	1.38
22	BA	2738	A	C8-N7	6.28	1.35	1.31
22	BA	2850	A	C5-C4	-6.28	1.34	1.38
1	AA	1254	A	C5-C4	-6.28	1.34	1.38
1	AA	1433	A	C5-C4	-6.28	1.34	1.38
1	AA	78	A	C5-C4	-6.28	1.34	1.38
22	BA	626	A	C5-C4	-6.28	1.34	1.38
22	BA	1470	A	N3-C4	6.28	1.38	1.34
22	BA	1591	A	C5-C4	-6.28	1.34	1.38
22	BA	1780	A	C5-C4	-6.28	1.34	1.38
1	AA	28	A	C5-C4	-6.28	1.34	1.38
1	AA	270	A	C5-C4	-6.28	1.34	1.38
1	AA	1362	A	C5-C4	-6.28	1.34	1.38
22	BA	324	A	C8-N7	6.28	1.35	1.31
55	B8	21	A	C8-N7	6.28	1.35	1.31
1	AA	1155	A	C5-C4	-6.27	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1073	A	C5-C4	-6.27	1.34	1.38
23	BB	45	A	C5-C4	-6.27	1.34	1.38
1	AA	1111	A	C5-C4	-6.27	1.34	1.38
22	BA	320	A	C5-C4	-6.27	1.34	1.38
22	BA	1385	A	C8-N7	6.27	1.35	1.31
22	BA	2198	A	N3-C4	6.27	1.38	1.34
22	BA	896	A	N3-C4	6.27	1.38	1.34
23	BB	50	A	C5-C4	-6.27	1.34	1.38
1	AA	131	A	C5-C4	-6.27	1.34	1.38
22	BA	1549	A	C8-N7	6.27	1.35	1.31
23	BB	53	A	C5-C4	-6.27	1.34	1.38
1	AA	16	A	C5-C4	-6.27	1.34	1.38
1	AA	728	A	C5-C4	-6.27	1.34	1.38
22	BA	1127	A	C8-N7	6.27	1.35	1.31
22	BA	1347	A	C8-N7	6.27	1.35	1.31
22	BA	1772	A	C8-N7	6.27	1.35	1.31
22	BA	2448	A	C8-N7	6.27	1.35	1.31
1	AA	415	A	N3-C4	6.27	1.38	1.34
22	BA	627	A	N3-C4	6.27	1.38	1.34
1	AA	192	A	N3-C4	6.26	1.38	1.34
1	AA	864	A	C5-C4	-6.26	1.34	1.38
22	BA	94	A	C5-C4	-6.26	1.34	1.38
22	BA	2734	A	C5-C4	-6.26	1.34	1.38
1	AA	1012	A	C5-C4	-6.26	1.34	1.38
1	AA	356	A	N3-C4	6.26	1.38	1.34
1	AA	938	A	C5-C4	-6.26	1.34	1.38
22	BA	217	A	C5-C4	-6.26	1.34	1.38
1	AA	1274	A	N3-C4	6.26	1.38	1.34
22	BA	2778	A	C8-N7	6.26	1.35	1.31
55	B8	59	A	C8-N7	6.26	1.35	1.31
1	AA	397	A	C5-C4	-6.26	1.34	1.38
1	AA	873	A	C8-N7	6.26	1.35	1.31
22	BA	1532	A	N3-C4	6.26	1.38	1.34
1	AA	478	A	N3-C4	6.26	1.38	1.34
22	BA	1304	A	C8-N7	6.26	1.35	1.31
1	AA	1179	A	N3-C4	6.25	1.38	1.34
22	BA	1384	A	C5-C4	-6.25	1.34	1.38
1	AA	325	A	C5-C4	-6.25	1.34	1.38
1	AA	563	A	C5-C4	-6.25	1.34	1.38
22	BA	300	A	C8-N7	6.25	1.35	1.31
22	BA	734	A	C8-N7	6.25	1.35	1.31
22	BA	849	A	C5-C4	-6.25	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2267	A	C5-C4	-6.25	1.34	1.38
1	AA	1167	A	N3-C4	6.25	1.38	1.34
22	BA	402	A	C8-N7	6.25	1.35	1.31
22	BA	2183	A	C5-C4	-6.25	1.34	1.38
22	BA	2821	A	C8-N7	6.25	1.35	1.31
1	AA	1146	A	N3-C4	6.25	1.38	1.34
1	AA	1534	A	N3-C4	6.25	1.38	1.34
1	AA	1285	A	C5-C4	-6.25	1.34	1.38
22	BA	429	A	C8-N7	6.25	1.35	1.31
22	BA	1395	A	C8-N7	6.25	1.35	1.31
22	BA	1598	A	C8-N7	6.25	1.35	1.31
22	BA	1717	A	C5-C4	-6.25	1.34	1.38
1	AA	155	A	C5-C4	-6.25	1.34	1.38
22	BA	689	A	C8-N7	6.25	1.35	1.31
22	BA	654	A	N3-C4	6.25	1.38	1.34
1	AA	1102	A	C5-C4	-6.24	1.34	1.38
22	BA	311	A	C5-C4	-6.24	1.34	1.38
22	BA	2170	A	N3-C4	6.24	1.38	1.34
22	BA	2273	A	N3-C4	6.24	1.38	1.34
22	BA	2297	A	C8-N7	6.24	1.35	1.31
22	BA	2572	A	C8-N7	6.24	1.35	1.31
1	AA	338	A	C5-C4	-6.24	1.34	1.38
1	AA	393	A	N3-C4	6.24	1.38	1.34
1	AA	1396	A	N3-C4	6.24	1.38	1.34
1	AA	696	A	C5-C4	-6.24	1.34	1.38
1	AA	949	A	C5-C4	-6.24	1.34	1.38
1	AA	1012	A	N3-C4	6.24	1.38	1.34
22	BA	63	A	C8-N7	6.24	1.35	1.31
22	BA	925	A	C8-N7	6.24	1.35	1.31
1	AA	964	A	C5-C4	-6.24	1.34	1.38
22	BA	1938	A	C8-N7	6.24	1.35	1.31
1	AA	1080	A	C5-C4	-6.24	1.34	1.38
22	BA	156	A	C5-C4	-6.23	1.34	1.38
1	AA	1093	A	C5-C4	-6.23	1.34	1.38
22	BA	2309	A	N3-C4	6.23	1.38	1.34
22	BA	2734	A	N3-C4	6.23	1.38	1.34
22	BA	2856	A	N3-C4	6.23	1.38	1.34
1	AA	553	A	N3-C4	6.23	1.38	1.34
22	BA	1569	A	C8-N7	6.23	1.35	1.31
22	BA	2813	A	N3-C4	6.23	1.38	1.34
23	BB	15	A	C5-C4	-6.23	1.34	1.38
1	AA	190	A	C8-N7	6.23	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1802	A	C5-C4	-6.23	1.34	1.38
22	BA	2448	A	C5-C4	-6.23	1.34	1.38
22	BA	845	A	C8-N7	6.23	1.35	1.31
22	BA	1285	A	C5-C4	-6.23	1.34	1.38
1	AA	640	A	N3-C4	6.22	1.38	1.34
1	AA	1180	A	N3-C4	6.22	1.38	1.34
22	BA	783	A	C8-N7	6.22	1.35	1.31
22	BA	1046	A	N3-C4	6.22	1.38	1.34
22	BA	1655	A	N3-C4	6.22	1.38	1.34
1	AA	66	A	C5-C4	-6.22	1.34	1.38
1	AA	197	A	N3-C4	6.22	1.38	1.34
1	AA	1204	A	C5-C4	-6.22	1.34	1.38
22	BA	2369	A	C8-N7	6.22	1.35	1.31
22	BA	142	A	C5-C4	-6.22	1.34	1.38
22	BA	538	A	C8-N7	6.22	1.35	1.31
22	BA	613	A	N3-C4	6.22	1.38	1.34
22	BA	2800	A	C5-C4	-6.22	1.34	1.38
55	B8	26	A	C8-N7	6.22	1.35	1.31
1	AA	246	A	N3-C4	6.22	1.38	1.34
1	AA	1152	A	N3-C4	6.22	1.38	1.34
22	BA	362	A	N3-C4	6.22	1.38	1.34
1	AA	749	A	N3-C4	6.21	1.38	1.34
22	BA	541	A	C8-N7	6.21	1.35	1.31
22	BA	1274	A	C8-N7	6.21	1.35	1.31
1	AA	174	A	N3-C4	6.21	1.38	1.34
1	AA	746	A	N3-C4	6.21	1.38	1.34
1	AA	649	A	C5-C4	-6.21	1.34	1.38
22	BA	430	A	C5-C4	-6.21	1.34	1.38
22	BA	2094	A	C5-C4	-6.21	1.34	1.38
22	BA	2882	A	N3-C4	6.21	1.38	1.34
22	BA	2799	A	C5-C4	-6.21	1.34	1.38
1	AA	1021	A	N3-C4	6.20	1.38	1.34
22	BA	2097	A	C5-C4	-6.20	1.34	1.38
1	AA	753	A	C5-C4	-6.20	1.34	1.38
1	AA	1196	A	N3-C4	6.20	1.38	1.34
22	BA	1919	A	C5-C4	-6.20	1.34	1.38
1	AA	908	A	C5-C4	-6.20	1.34	1.38
1	AA	1288	A	N3-C4	6.20	1.38	1.34
22	BA	483	A	C8-N7	6.20	1.35	1.31
22	BA	2070	A	C8-N7	6.20	1.35	1.31
22	BA	2225	A	C8-N7	6.20	1.35	1.31
23	BB	57	A	C5-C4	-6.20	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	195	A	C5-C4	-6.19	1.34	1.38
22	BA	503	A	C5-C4	-6.19	1.34	1.38
22	BA	1586	A	C5-C4	-6.19	1.34	1.38
1	AA	687	A	C5-C4	-6.19	1.34	1.38
1	AA	831	A	N3-C4	6.19	1.38	1.34
22	BA	661	A	C8-N7	6.19	1.35	1.31
22	BA	1021	A	C8-N7	6.19	1.35	1.31
22	BA	1490	A	C5-C4	-6.19	1.34	1.38
22	BA	1652	A	C8-N7	6.19	1.35	1.31
1	AA	300	A	N3-C4	6.19	1.38	1.34
1	AA	687	A	N3-C4	6.19	1.38	1.34
1	AA	996	A	C5-C4	-6.19	1.34	1.38
22	BA	2497	A	C5-C4	-6.19	1.34	1.38
1	AA	907	A	N3-C4	6.19	1.38	1.34
1	AA	1046	A	N3-C4	6.19	1.38	1.34
22	BA	73	A	C5-C4	-6.19	1.34	1.38
1	AA	250	A	N3-C4	6.19	1.38	1.34
1	AA	1145	A	C5-C4	-6.19	1.34	1.38
22	BA	2753	A	N3-C4	6.19	1.38	1.34
1	AA	630	A	C5-C4	-6.19	1.34	1.38
1	AA	1437	A	N3-C4	6.19	1.38	1.34
22	BA	172	A	C5-C4	-6.19	1.34	1.38
22	BA	1070	A	N3-C4	6.19	1.38	1.34
22	BA	1328	A	C8-N7	6.19	1.35	1.31
1	AA	1374	A	C5-C4	-6.18	1.34	1.38
22	BA	1205	A	C5-C4	-6.18	1.34	1.38
22	BA	2095	A	C5-C4	-6.18	1.34	1.38
22	BA	2335	A	C8-N7	6.18	1.35	1.31
1	AA	329	A	C5-C4	-6.18	1.34	1.38
1	AA	781	A	N3-C4	6.18	1.38	1.34
1	AA	949	A	N3-C4	6.18	1.38	1.34
1	AA	1004	A	C5-C4	-6.18	1.34	1.38
1	AA	560	A	N3-C4	6.18	1.38	1.34
22	BA	165	A	C5-C4	-6.18	1.34	1.38
1	AA	815	A	C5-C4	-6.18	1.34	1.38
22	BA	1342	A	C8-N7	6.18	1.35	1.31
23	BB	66	A	C5-C4	-6.18	1.34	1.38
1	AA	704	A	C5-C4	-6.18	1.34	1.38
22	BA	2426	A	C8-N7	6.18	1.35	1.31
22	BA	2388	A	C5-C4	-6.17	1.34	1.38
22	BA	2813	A	C8-N7	6.17	1.35	1.31
22	BA	941	A	C8-N7	6.17	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	52	A	N3-C4	6.17	1.38	1.34
1	AA	1169	A	N3-C4	6.17	1.38	1.34
1	AA	199	A	N3-C4	6.17	1.38	1.34
1	AA	466	A	N3-C4	6.17	1.38	1.34
22	BA	1998	A	C8-N7	6.17	1.35	1.31
22	BA	2088	A	C8-N7	6.17	1.35	1.31
1	AA	495	A	N3-C4	6.17	1.38	1.34
22	BA	1393	A	C8-N7	6.17	1.35	1.31
22	BA	2598	A	C8-N7	6.17	1.35	1.31
1	AA	65	A	C5-C4	-6.17	1.34	1.38
1	AA	1151	A	C5-C4	-6.17	1.34	1.38
1	AA	1333	A	C5-C4	-6.17	1.34	1.38
22	BA	751	A	N3-C4	6.17	1.38	1.34
22	BA	1553	A	N3-C4	6.17	1.38	1.34
1	AA	1248	A	N3-C4	6.16	1.38	1.34
22	BA	190	A	C5-C4	-6.16	1.34	1.38
22	BA	219	A	C8-N7	6.16	1.35	1.31
22	BA	878	A	N3-C4	6.16	1.38	1.34
1	AA	1042	A	N3-C4	6.16	1.38	1.34
1	AA	1167	A	C5-C4	-6.16	1.34	1.38
22	BA	547	A	N3-C4	6.16	1.38	1.34
1	AA	729	A	C5-C4	-6.16	1.34	1.38
1	AA	1256	A	N3-C4	6.16	1.38	1.34
22	BA	2042	A	C8-N7	6.16	1.35	1.31
1	AA	81	A	N3-C4	6.16	1.38	1.34
22	BA	1373	A	C5-C4	-6.16	1.34	1.38
1	AA	72	A	N3-C4	6.16	1.38	1.34
1	AA	174	A	C5-C4	-6.16	1.34	1.38
1	AA	1110	A	C5-C4	-6.16	1.34	1.38
22	BA	819	A	C5-C4	-6.16	1.34	1.38
22	BA	1508	A	N3-C4	6.16	1.38	1.34
22	BA	2711	A	C5-C4	-6.15	1.34	1.38
1	AA	1044	A	C5-C4	-6.15	1.34	1.38
22	BA	960	A	C5-C4	-6.15	1.34	1.38
22	BA	1050	A	C5-C4	-6.15	1.34	1.38
22	BA	1469	A	C8-N7	6.15	1.35	1.31
22	BA	877	A	C5-C4	-6.15	1.34	1.38
22	BA	1001	A	C8-N7	6.15	1.35	1.31
22	BA	1151	A	C8-N7	6.15	1.35	1.31
22	BA	1772	A	N3-C4	6.15	1.38	1.34
22	BA	2461	A	C8-N7	6.15	1.35	1.31
22	BA	2518	A	N3-C4	6.15	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	207	A	C8-N7	6.15	1.35	1.31
1	AA	1246	A	C5-C4	-6.15	1.34	1.38
22	BA	1244	A	N3-C4	6.15	1.38	1.34
22	BA	1586	A	N3-C4	6.15	1.38	1.34
22	BA	2014	A	C5-C4	-6.15	1.34	1.38
22	BA	2602	A	C5-C4	-6.15	1.34	1.38
1	AA	336	A	N3-C4	6.14	1.38	1.34
22	BA	340	A	C5-C4	-6.14	1.34	1.38
22	BA	176	A	N3-C4	6.14	1.38	1.34
22	BA	1744	A	N3-C4	6.14	1.38	1.34
1	AA	451	A	C5-C4	-6.14	1.34	1.38
22	BA	2577	A	C8-N7	6.14	1.35	1.31
22	BA	477	A	C8-N7	6.14	1.35	1.31
22	BA	1815	A	C8-N7	6.14	1.35	1.31
1	AA	496	A	C5-C4	-6.14	1.34	1.38
1	AA	969	A	C5-C4	-6.14	1.34	1.38
1	AA	1180	A	C5-C4	-6.14	1.34	1.38
22	BA	142	A	N3-C4	6.14	1.38	1.34
1	AA	152	A	C5-C4	-6.13	1.34	1.38
1	AA	1246	A	N3-C4	6.13	1.38	1.34
1	AA	1396	A	C5-C4	-6.13	1.34	1.38
22	BA	677	A	N3-C4	6.13	1.38	1.34
22	BA	750	A	N3-C4	6.13	1.38	1.34
22	BA	1067	A	N3-C4	6.13	1.38	1.34
22	BA	1420	A	C5-C4	-6.13	1.34	1.38
22	BA	1591	A	N3-C4	6.13	1.38	1.34
1	AA	327	A	N3-C4	6.13	1.38	1.34
1	AA	435	A	N3-C4	6.13	1.38	1.34
1	AA	461	A	C2-N3	6.13	1.39	1.33
1	AA	1171	A	N3-C4	6.13	1.38	1.34
1	AA	1225	A	C5-C4	-6.13	1.34	1.38
22	BA	1403	A	C8-N7	6.13	1.35	1.31
22	BA	1735	A	C5-C4	-6.13	1.34	1.38
22	BA	2482	A	C8-N7	6.13	1.35	1.31
1	AA	509	A	C5-C4	-6.13	1.34	1.38
22	BA	10	A	C5-C4	-6.13	1.34	1.38
22	BA	118	A	C8-N7	6.13	1.35	1.31
22	BA	2634	A	C8-N7	6.13	1.35	1.31
1	AA	414	A	C5-C4	-6.13	1.34	1.38
1	AA	608	A	N3-C4	6.13	1.38	1.34
1	AA	1225	A	N3-C4	6.13	1.38	1.34
1	AA	1493	A	C5-C4	-6.13	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	176	A	C8-N7	6.13	1.35	1.31
1	AA	1019	A	C5-C4	-6.12	1.34	1.38
1	AA	532	A	N3-C4	6.12	1.38	1.34
22	BA	371	A	C5-C4	-6.12	1.34	1.38
22	BA	1701	A	N3-C4	6.12	1.38	1.34
55	B8	66	A	N3-C4	6.12	1.38	1.34
1	AA	59	A	N3-C4	6.12	1.38	1.34
22	BA	1805	A	C8-N7	6.12	1.35	1.31
1	AA	974	A	C5-C4	-6.12	1.34	1.38
22	BA	833	A	C8-N7	6.12	1.35	1.31
1	AA	1170	A	N3-C4	6.12	1.38	1.34
1	AA	262	A	N3-C4	6.12	1.38	1.34
1	AA	1236	A	C5-C4	-6.12	1.34	1.38
22	BA	2108	A	N3-C4	6.12	1.38	1.34
22	BA	2660	A	C5-C4	-6.12	1.34	1.38
1	AA	397	A	N3-C4	6.11	1.38	1.34
1	AA	1082	A	C5-C4	-6.11	1.34	1.38
22	BA	505	A	C8-N7	6.11	1.35	1.31
22	BA	2725	A	C8-N7	6.11	1.35	1.31
23	BB	39	A	N3-C4	6.11	1.38	1.34
1	AA	205	A	N3-C4	6.11	1.38	1.34
22	BA	2171	A	C5-C4	-6.11	1.34	1.38
55	B8	73	A	N3-C4	6.11	1.38	1.34
1	AA	496	A	N3-C4	6.11	1.38	1.34
1	AA	499	A	N3-C4	6.11	1.38	1.34
1	AA	1363	A	N3-C4	6.11	1.38	1.34
22	BA	2814	A	C5-C4	-6.11	1.34	1.38
1	AA	55	A	N3-C4	6.11	1.38	1.34
22	BA	752	A	C5-C4	-6.11	1.34	1.38
22	BA	2657	A	C5-C4	-6.11	1.34	1.38
1	AA	152	A	N3-C4	6.11	1.38	1.34
1	AA	819	A	C5-C4	-6.11	1.34	1.38
22	BA	892	A	N3-C4	6.11	1.38	1.34
22	BA	1794	A	C8-N7	6.11	1.35	1.31
1	AA	635	A	C5-C4	-6.11	1.34	1.38
1	AA	1191	A	N3-C4	6.11	1.38	1.34
22	BA	345	A	C5-C4	-6.11	1.34	1.38
22	BA	742	A	C8-N7	6.11	1.35	1.31
22	BA	1133	A	C5-C4	-6.11	1.34	1.38
22	BA	1866	A	C5-C4	-6.11	1.34	1.38
1	AA	366	A	C5-C4	-6.10	1.34	1.38
1	AA	673	A	N3-C4	6.10	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	889	A	C5-C4	-6.10	1.34	1.38
1	AA	1346	A	C5-C4	-6.10	1.34	1.38
22	BA	1103	A	N3-C4	6.10	1.38	1.34
1	AA	1257	A	C5-C4	-6.10	1.34	1.38
22	BA	1265	A	C5-C4	-6.10	1.34	1.38
1	AA	263	A	C5-C4	-6.10	1.34	1.38
1	AA	465	A	N3-C4	6.10	1.38	1.34
1	AA	300	A	C5-C4	-6.10	1.34	1.38
22	BA	1275	A	C8-N7	6.10	1.35	1.31
22	BA	2352	A	C5-C4	-6.10	1.34	1.38
1	AA	642	A	C5-C4	-6.10	1.34	1.38
1	AA	1014	A	N3-C4	6.10	1.38	1.34
22	BA	73	A	C8-N7	6.10	1.35	1.31
22	BA	676	A	C8-N7	6.10	1.35	1.31
22	BA	699	A	C5-C4	-6.10	1.34	1.38
22	BA	1085	A	C5-C4	-6.10	1.34	1.38
22	BA	1590	A	C5-C4	-6.10	1.34	1.38
1	AA	250	A	C5-C4	-6.09	1.34	1.38
1	AA	1021	A	C5-C4	-6.09	1.34	1.38
1	AA	1324	A	N3-C4	6.09	1.38	1.34
22	BA	1151	A	N3-C4	6.09	1.38	1.34
22	BA	2268	A	C8-N7	6.09	1.35	1.31
1	AA	161	A	N3-C4	6.09	1.38	1.34
1	AA	1022	A	C5-C4	-6.09	1.34	1.38
1	AA	1150	A	N3-C4	6.09	1.38	1.34
22	BA	1254	A	C8-N7	6.09	1.35	1.31
1	AA	182	A	N3-C4	6.09	1.38	1.34
1	AA	282	A	C5-C4	-6.09	1.34	1.38
1	AA	676	A	N3-C4	6.09	1.38	1.34
22	BA	52	A	C5-C4	-6.09	1.34	1.38
22	BA	118	A	N3-C4	6.09	1.38	1.34
22	BA	1762	A	C8-N7	6.09	1.35	1.31
1	AA	189	A	N3-C4	6.09	1.38	1.34
1	AA	1044	A	N3-C4	6.09	1.38	1.34
22	BA	218	A	C8-N7	6.09	1.35	1.31
1	AA	182	A	C5-C4	-6.09	1.34	1.38
1	AA	533	A	C5-C4	-6.09	1.34	1.38
1	AA	547	A	C5-C4	-6.09	1.34	1.38
22	BA	1876	A	N3-C4	6.09	1.38	1.34
22	BA	2407	A	C8-N7	6.09	1.35	1.31
22	BA	2868	A	N3-C4	6.09	1.38	1.34
1	AA	412	A	C5-C4	-6.08	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	780	A	C5-C4	-6.08	1.34	1.38
1	AA	1046	A	C2-N3	6.08	1.39	1.33
1	AA	1197	A	C5-C4	-6.08	1.34	1.38
22	BA	1808	A	C5-C4	-6.08	1.34	1.38
23	BB	101	A	C2-N3	6.08	1.39	1.33
1	AA	749	A	C5-C4	-6.08	1.34	1.38
1	AA	1005	A	N3-C4	6.08	1.38	1.34
22	BA	101	A	C8-N7	6.08	1.35	1.31
22	BA	2860	A	C5-C4	-6.08	1.34	1.38
1	AA	2	A	N3-C4	6.08	1.38	1.34
22	BA	984	A	N3-C4	6.08	1.38	1.34
1	AA	747	A	N3-C4	6.08	1.38	1.34
22	BA	633	A	N3-C4	6.08	1.38	1.34
22	BA	1787	A	N3-C4	6.08	1.38	1.34
22	BA	2211	A	C5-C4	-6.08	1.34	1.38
1	AA	262	A	C5-C4	-6.08	1.34	1.38
1	AA	595	A	C5-C4	-6.08	1.34	1.38
1	AA	958	A	C5-C4	-6.08	1.34	1.38
1	AA	1092	A	C5-C4	-6.08	1.34	1.38
1	AA	1105	A	C5-C4	-6.08	1.34	1.38
22	BA	141	G	N7-C5	6.08	1.42	1.39
1	AA	487	A	N3-C4	6.08	1.38	1.34
1	AA	1105	A	N3-C4	6.08	1.38	1.34
22	BA	1785	A	C5-C4	-6.08	1.34	1.38
55	B8	42	A	C5-C4	-6.08	1.34	1.38
22	BA	299	A	C8-N7	6.07	1.35	1.31
22	BA	1077	A	C5-C4	-6.07	1.34	1.38
22	BA	1413	A	C5-C4	-6.07	1.34	1.38
22	BA	1583	A	N3-C4	6.07	1.38	1.34
22	BA	2748	A	N3-C4	6.07	1.38	1.34
1	AA	179	A	N3-C4	6.07	1.38	1.34
23	BB	101	A	C8-N7	6.07	1.35	1.31
1	AA	695	A	C5-C4	-6.07	1.34	1.38
22	BA	2274	A	C8-N7	6.07	1.35	1.31
22	BA	2665	A	N3-C4	6.07	1.38	1.34
1	AA	1311	A	C5-C4	-6.07	1.34	1.38
22	BA	1029	A	N3-C4	6.07	1.38	1.34
22	BA	2513	A	C5-C4	-6.07	1.34	1.38
1	AA	50	A	C5-C4	-6.07	1.34	1.38
1	AA	1152	A	C5-C4	-6.07	1.34	1.38
1	AA	1531	A	N3-C4	6.07	1.38	1.34
22	BA	1668	A	C8-N7	6.07	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2101	A	C5-C4	-6.07	1.34	1.38
22	BA	1069	A	C5-C4	-6.07	1.34	1.38
1	AA	167	A	C5-C4	-6.06	1.34	1.38
22	BA	2080	A	C8-N7	6.06	1.35	1.31
22	BA	792	A	N3-C4	6.06	1.38	1.34
22	BA	1308	A	C8-N7	6.06	1.35	1.31
1	AA	535	A	C5-C4	-6.06	1.34	1.38
1	AA	1254	A	N3-C4	6.06	1.38	1.34
22	BA	2766	A	C8-N7	6.06	1.35	1.31
1	AA	831	A	C5-C4	-6.06	1.34	1.38
22	BA	270	A	C5-C4	-6.06	1.34	1.38
22	BA	756	A	N3-C4	6.06	1.38	1.34
22	BA	1936	A	N3-C4	6.06	1.38	1.34
22	BA	1689	A	C8-N7	6.06	1.35	1.31
1	AA	1036	A	C5-C4	-6.05	1.34	1.38
22	BA	1722	A	C5-C4	-6.05	1.34	1.38
22	BA	2590	A	C8-N7	6.05	1.35	1.31
1	AA	1169	A	C5-C4	-6.05	1.34	1.38
1	AA	1269	A	N3-C4	6.05	1.38	1.34
1	AA	1360	A	C5-C4	-6.05	1.34	1.38
22	BA	63	A	N3-C4	6.05	1.38	1.34
22	BA	1237	A	C5-C4	-6.05	1.34	1.38
22	BA	1307	A	C8-N7	6.05	1.35	1.31
1	AA	189	A	C5-C4	-6.05	1.34	1.38
22	BA	631	A	N3-C4	6.05	1.38	1.34
22	BA	2317	A	N3-C4	6.05	1.38	1.34
1	AA	315	A	N3-C4	6.05	1.38	1.34
22	BA	507	A	N3-C4	6.05	1.38	1.34
1	AA	1311	A	N3-C4	6.05	1.38	1.34
22	BA	689	A	N3-C4	6.05	1.38	1.34
1	AA	1155	A	N3-C4	6.04	1.38	1.34
1	AA	1480	A	C5-C4	-6.04	1.34	1.38
1	AA	171	A	C5-C4	-6.04	1.34	1.38
1	AA	279	A	C5-C4	-6.04	1.34	1.38
1	AA	432	A	C5-C4	-6.04	1.34	1.38
22	BA	501	A	C8-N7	6.04	1.35	1.31
22	BA	1237	A	N3-C4	6.04	1.38	1.34
22	BA	2101	A	N3-C4	6.04	1.38	1.34
22	BA	2758	A	C5-C4	-6.04	1.34	1.38
1	AA	622	A	C5-C4	-6.04	1.34	1.38
22	BA	1142	A	C8-N7	6.04	1.35	1.31
1	AA	98	A	C5-C4	-6.04	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1092	A	N3-C4	6.04	1.38	1.34
22	BA	38	A	C8-N7	6.04	1.35	1.31
22	BA	1772	A	C5-C4	-6.04	1.34	1.38
22	BA	1090	A	C5-C4	-6.04	1.34	1.38
22	BA	2478	A	N3-C4	6.04	1.38	1.34
22	BA	91	A	C5-C4	-6.04	1.34	1.38
22	BA	368	A	C5-C4	-6.04	1.34	1.38
22	BA	2309	A	C5-C4	-6.04	1.34	1.38
1	AA	1271	A	C5-C4	-6.03	1.34	1.38
22	BA	347	A	N3-C4	6.03	1.38	1.34
22	BA	2097	A	N3-C4	6.03	1.38	1.34
1	AA	344	A	N3-C4	6.03	1.38	1.34
1	AA	393	A	C5-C4	-6.03	1.34	1.38
1	AA	460	A	C5-C4	-6.03	1.34	1.38
22	BA	1274	A	N3-C4	6.03	1.38	1.34
22	BA	2119	A	C5-C4	-6.03	1.34	1.38
22	BA	2453	A	N3-C4	6.03	1.38	1.34
22	BA	2792	A	N3-C4	6.03	1.38	1.34
1	AA	547	A	N3-C4	6.03	1.38	1.34
22	BA	1089	A	C5-C4	-6.03	1.34	1.38
22	BA	1413	A	N3-C4	6.03	1.38	1.34
22	BA	2158	A	C5-C4	-6.03	1.34	1.38
1	AA	1055	A	C5-C4	-6.03	1.34	1.38
22	BA	513	A	N3-C4	6.03	1.38	1.34
22	BA	2336	A	C8-N7	6.03	1.35	1.31
22	BA	2614	A	C8-N7	6.03	1.35	1.31
1	AA	1261	A	C5-C4	-6.02	1.34	1.38
1	AA	1289	A	N3-C4	6.02	1.38	1.34
1	AA	1375	A	N3-C4	6.02	1.38	1.34
22	BA	2418	A	C8-N7	6.02	1.35	1.31
1	AA	1014	A	C5-C4	-6.02	1.34	1.38
22	BA	1966	A	C8-N7	6.02	1.35	1.31
1	AA	1500	A	N3-C4	6.02	1.38	1.34
1	AA	430	A	C5-C4	-6.02	1.34	1.38
1	AA	655	A	N3-C4	6.02	1.38	1.34
22	BA	1490	A	N3-C4	6.02	1.38	1.34
22	BA	1713	A	N3-C4	6.02	1.38	1.34
22	BA	2135	A	N3-C4	6.02	1.38	1.34
22	BA	2542	A	C8-N7	6.02	1.35	1.31
1	AA	205	A	C5-C4	-6.02	1.34	1.38
1	AA	900	A	C8-N7	6.02	1.35	1.31
1	AA	1176	A	C5-C4	-6.02	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1641	A	C8-N7	6.02	1.35	1.31
22	BA	1722	A	N3-C4	6.02	1.38	1.34
22	BA	2051	A	C8-N7	6.02	1.35	1.31
22	BA	2482	A	N3-C4	6.02	1.38	1.34
1	AA	1394	A	N3-C4	6.02	1.38	1.34
22	BA	466	A	C8-N7	6.02	1.35	1.31
1	AA	199	A	C5-C4	-6.01	1.34	1.38
1	AA	696	A	N3-C4	6.01	1.38	1.34
22	BA	2142	A	C2-N3	6.01	1.39	1.33
22	BA	1144	A	C8-N7	6.01	1.35	1.31
1	AA	579	A	C5-C4	-6.01	1.34	1.38
1	AA	694	A	N3-C4	6.01	1.38	1.34
1	AA	702	A	C5-C4	-6.01	1.34	1.38
1	AA	1441	A	C5-C4	-6.01	1.34	1.38
1	AA	162	A	N3-C4	6.01	1.38	1.34
22	BA	2287	A	N3-C4	6.01	1.38	1.34
1	AA	32	A	N3-C4	6.01	1.38	1.34
1	AA	1067	A	C5-C4	-6.01	1.34	1.38
1	AA	1188	A	C5-C4	-6.01	1.34	1.38
22	BA	382	A	N3-C4	6.01	1.38	1.34
22	BA	616	A	N3-C4	6.01	1.38	1.34
22	BA	878	A	C5-C4	-6.01	1.34	1.38
22	BA	896	A	C5-C4	-6.01	1.34	1.38
22	BA	1590	A	N3-C4	6.01	1.38	1.34
1	AA	253	A	N3-C4	6.00	1.38	1.34
1	AA	282	A	N3-C4	6.00	1.38	1.34
1	AA	77	A	C5-C4	-6.00	1.34	1.38
1	AA	162	A	C5-C4	-6.00	1.34	1.38
22	BA	262	A	C8-N7	6.00	1.35	1.31
22	BA	384	A	C8-N7	6.00	1.35	1.31
22	BA	918	A	C8-N7	6.00	1.35	1.31
22	BA	1871	A	C5-C4	-6.00	1.34	1.38
22	BA	2534	A	C5-C4	-6.00	1.34	1.38
1	AA	635	A	N3-C4	6.00	1.38	1.34
1	AA	1004	A	N3-C4	6.00	1.38	1.34
22	BA	2851	A	C8-N7	6.00	1.35	1.31
1	AA	959	A	C5-C4	-6.00	1.34	1.38
22	BA	1987	A	N3-C4	6.00	1.38	1.34
1	AA	195	A	C5-C4	-6.00	1.34	1.38
22	BA	195	A	N3-C4	6.00	1.38	1.34
22	BA	1900	A	C5-C4	-6.00	1.34	1.38
1	AA	101	A	C5-C4	-6.00	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	5	A	N3-C4	6.00	1.38	1.34
22	BA	863	A	C8-N7	6.00	1.35	1.31
22	BA	1050	A	N3-C4	6.00	1.38	1.34
22	BA	1420	A	N3-C4	6.00	1.38	1.34
22	BA	2117	A	C5-C4	-6.00	1.34	1.38
22	BA	73	A	N3-C4	6.00	1.38	1.34
22	BA	203	A	C8-N7	6.00	1.35	1.31
22	BA	2531	A	N3-C4	6.00	1.38	1.34
1	AA	983	A	C5-C4	-5.99	1.34	1.38
22	BA	2868	A	C8-N7	5.99	1.35	1.31
1	AA	139	A	C5-C4	-5.99	1.34	1.38
1	AA	996	A	N3-C4	5.99	1.38	1.34
22	BA	472	A	C8-N7	5.99	1.35	1.31
22	BA	2654	A	N3-C4	5.99	1.38	1.34
1	AA	243	A	N3-C4	5.99	1.38	1.34
22	BA	38	A	N3-C4	5.99	1.38	1.34
22	BA	1477	A	N3-C4	5.99	1.38	1.34
22	BA	2082	A	C5-C4	-5.99	1.34	1.38
1	AA	1508	A	C5-C4	-5.99	1.34	1.38
22	BA	789	A	C8-N7	5.99	1.35	1.31
22	BA	2753	A	C5-C4	-5.99	1.34	1.38
1	AA	609	A	N3-C4	5.99	1.38	1.34
1	AA	1250	A	C5-C4	-5.99	1.34	1.38
22	BA	849	A	C8-N7	5.99	1.35	1.31
1	AA	374	A	N3-C4	5.99	1.38	1.34
22	BA	203	A	C5-C4	-5.99	1.34	1.38
22	BA	354	A	C5-C4	-5.99	1.34	1.38
22	BA	990	A	N3-C4	5.99	1.38	1.34
1	AA	451	A	N3-C4	5.98	1.38	1.34
1	AA	706	A	C5-C4	-5.98	1.34	1.38
22	BA	1453	A	N3-C4	5.98	1.38	1.34
22	BA	1580	A	C5-C4	-5.98	1.34	1.38
22	BA	2142	A	C5-C4	-5.98	1.34	1.38
22	BA	2184	A	C5-C4	-5.98	1.34	1.38
55	B8	69	A	C5-C4	-5.98	1.34	1.38
1	AA	596	A	N3-C4	5.98	1.38	1.34
1	AA	1251	A	C5-C4	-5.98	1.34	1.38
22	BA	743	A	C8-N7	5.98	1.35	1.31
22	BA	1494	A	C5-C4	-5.98	1.34	1.38
1	AA	139	A	N3-C4	5.98	1.38	1.34
1	AA	1456	A	C5-C4	-5.98	1.34	1.38
1	AA	71	A	N3-C4	5.98	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	131	A	C8-N7	5.98	1.35	1.31
1	AA	901	A	C5-C4	-5.98	1.34	1.38
1	AA	1146	A	C5-C4	-5.97	1.34	1.38
1	AA	1216	A	C5-C4	-5.97	1.34	1.38
1	AA	1251	A	N3-C4	5.97	1.38	1.34
1	AA	923	A	N3-C4	5.97	1.38	1.34
1	AA	977	A	C5-C4	-5.97	1.34	1.38
22	BA	592	A	C8-N7	5.97	1.35	1.31
22	BA	1069	A	N3-C4	5.97	1.38	1.34
22	BA	2530	A	C5-C4	-5.97	1.34	1.38
1	AA	190	A	N3-C4	5.97	1.38	1.34
1	AA	1248	A	C5-C4	-5.97	1.34	1.38
1	AA	71	A	C5-C4	-5.97	1.34	1.38
1	AA	181	A	N3-C4	5.97	1.38	1.34
1	AA	790	A	C5-C4	-5.97	1.34	1.38
22	BA	226	A	C8-N7	5.97	1.35	1.31
22	BA	270	A	N3-C4	5.97	1.38	1.34
22	BA	1155	A	N3-C4	5.97	1.38	1.34
1	AA	1374	A	N3-C4	5.97	1.38	1.34
22	BA	346	A	N3-C4	5.97	1.38	1.34
1	AA	865	A	C5-C4	-5.97	1.34	1.38
22	BA	1739	A	N3-C4	5.97	1.38	1.34
22	BA	1848	A	N3-C4	5.97	1.38	1.34
22	BA	2288	A	N3-C4	5.97	1.38	1.34
22	BA	2887	A	N3-C4	5.96	1.38	1.34
22	BA	1809	A	C8-N7	5.96	1.35	1.31
1	AA	460	A	N3-C4	5.96	1.38	1.34
1	AA	1216	A	N3-C4	5.96	1.38	1.34
1	AA	1219	A	C5-C4	-5.96	1.34	1.38
22	BA	2725	A	N3-C4	5.96	1.38	1.34
22	BA	2886	A	C8-N7	5.96	1.35	1.31
1	AA	938	A	N3-C4	5.96	1.38	1.34
1	AA	414	A	N3-C4	5.96	1.38	1.34
22	BA	900	A	N3-C4	5.96	1.38	1.34
22	BA	1608	A	C8-N7	5.96	1.35	1.31
22	BA	2014	A	C8-N7	5.96	1.35	1.31
22	BA	2059	A	C5-C4	-5.96	1.34	1.38
22	BA	1365	A	C8-N7	5.96	1.35	1.31
22	BA	53	A	N3-C4	5.96	1.38	1.34
22	BA	152	A	N3-C4	5.96	1.38	1.34
22	BA	1085	A	N3-C4	5.95	1.38	1.34
22	BA	1953	A	C8-N7	5.95	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	935	A	N3-C4	5.95	1.38	1.34
1	AA	130	A	N3-C4	5.95	1.38	1.34
1	AA	502	A	N3-C4	5.95	1.38	1.34
22	BA	1583	A	C5-C4	-5.95	1.34	1.38
22	BA	1616	A	C8-N7	5.95	1.35	1.31
22	BA	2700	A	C8-N7	5.95	1.35	1.31
1	AA	994	A	C5-C4	-5.95	1.34	1.38
22	BA	928	A	N3-C4	5.95	1.38	1.34
22	BA	2077	A	C5-C4	-5.95	1.34	1.38
22	BA	362	A	C5-C4	-5.95	1.34	1.38
1	AA	675	A	N3-C4	5.95	1.38	1.34
22	BA	739	A	C8-N7	5.95	1.35	1.31
55	B8	38	A	C8-N7	5.95	1.35	1.31
1	AA	695	A	N3-C4	5.94	1.38	1.34
22	BA	1535	A	N3-C4	5.94	1.38	1.34
22	BA	2114	A	C5-C4	-5.94	1.34	1.38
23	BB	73	A	N3-C4	5.94	1.38	1.34
1	AA	1201	A	C2-N3	5.94	1.38	1.33
22	BA	829	A	C8-N7	5.94	1.35	1.31
1	AA	468	A	C5-C4	-5.94	1.34	1.38
22	BA	165	A	N3-C4	5.94	1.38	1.34
1	AA	607	A	C5-C4	-5.94	1.34	1.38
22	BA	602	A	N3-C4	5.94	1.38	1.34
22	BA	1098	A	C5-C4	-5.94	1.34	1.38
1	AA	872	A	C5-C4	-5.94	1.34	1.38
1	AA	1410	A	N3-C4	5.94	1.38	1.34
22	BA	279	A	N3-C4	5.94	1.38	1.34
22	BA	2268	A	N3-C4	5.94	1.38	1.34
22	BA	2513	A	N3-C4	5.94	1.38	1.34
1	AA	1306	A	C5-C4	-5.93	1.34	1.38
1	AA	1349	A	N3-C4	5.93	1.38	1.34
22	BA	1745	A	N3-C4	5.93	1.38	1.34
22	BA	1872	A	N3-C4	5.93	1.38	1.34
1	AA	1239	A	N3-C4	5.93	1.38	1.34
22	BA	547	A	C5-C4	-5.93	1.34	1.38
22	BA	613	A	C5-C4	-5.93	1.34	1.38
22	BA	2566	A	N3-C4	5.93	1.38	1.34
22	BA	1302	A	C8-N7	5.93	1.35	1.31
22	BA	1665	A	N3-C4	5.93	1.38	1.34
1	AA	704	A	N3-C4	5.93	1.38	1.34
1	AA	901	A	N7-C5	-5.93	1.35	1.39
22	BA	354	A	N3-C4	5.93	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	603	A	N3-C4	5.93	1.38	1.34
22	BA	1322	A	N3-C4	5.93	1.38	1.34
22	BA	1548	A	N3-C4	5.93	1.38	1.34
22	BA	2082	A	C8-N7	5.93	1.35	1.31
1	AA	65	A	N3-C4	5.93	1.38	1.34
1	AA	430	A	N3-C4	5.93	1.38	1.34
1	AA	1016	A	C5-C4	-5.93	1.34	1.38
22	BA	1133	A	C8-N7	5.93	1.35	1.31
22	BA	1829	A	C8-N7	5.93	1.35	1.31
22	BA	2311	A	N3-C4	5.93	1.38	1.34
1	AA	363	A	C5-C4	-5.92	1.34	1.38
1	AA	1349	A	C5-C4	-5.92	1.34	1.38
1	AA	1368	A	C5-C4	-5.92	1.34	1.38
22	BA	344	A	N3-C4	5.92	1.38	1.34
22	BA	1901	A	C5-C4	-5.92	1.34	1.38
22	BA	2837	A	C8-N7	5.92	1.35	1.31
22	BA	1088	A	C5-C4	-5.92	1.34	1.38
22	BA	2883	A	N3-C4	5.92	1.38	1.34
1	AA	718	A	N3-C4	5.92	1.38	1.34
23	BB	99	A	C8-N7	5.92	1.35	1.31
1	AA	306	A	N3-C4	5.92	1.38	1.34
22	BA	1276	A	C8-N7	5.92	1.35	1.31
22	BA	2176	A	N3-C4	5.92	1.38	1.34
1	AA	539	A	C5-C4	-5.92	1.34	1.38
1	AA	1306	A	N3-C4	5.92	1.38	1.34
22	BA	1287	A	N3-C4	5.92	1.38	1.34
1	AA	487	A	C5-C4	-5.91	1.34	1.38
1	AA	1329	A	N3-C4	5.91	1.38	1.34
1	AA	1531	A	C5-C4	-5.91	1.34	1.38
1	AA	98	A	N3-C4	5.91	1.38	1.34
22	BA	1669	A	C5-C4	-5.91	1.34	1.38
54	B7	9	A	C5-C4	-5.91	1.34	1.38
1	AA	1197	A	N3-C4	5.91	1.38	1.34
22	BA	2287	A	C8-N7	5.91	1.35	1.31
22	BA	2682	A	N3-C4	5.91	1.38	1.34
1	AA	155	A	N3-C4	5.91	1.38	1.34
1	AA	374	A	C5-C4	-5.91	1.34	1.38
1	AA	1288	A	C5-C4	-5.91	1.34	1.38
1	AA	1357	A	C5-C4	-5.91	1.34	1.38
22	BA	632	A	C8-N7	5.91	1.35	1.31
1	AA	1252	A	C5-C4	-5.90	1.34	1.38
22	BA	1877	A	N3-C4	5.90	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1981	A	C8-N7	5.90	1.35	1.31
22	BA	2602	A	N3-C4	5.90	1.38	1.34
1	AA	1238	A	C5-C4	-5.90	1.34	1.38
22	BA	492	A	N3-C4	5.90	1.38	1.34
22	BA	1469	A	C5-C4	-5.90	1.34	1.38
22	BA	2003	A	C8-N7	5.90	1.35	1.31
22	BA	2679	A	C8-N7	5.90	1.35	1.31
22	BA	2851	A	N3-C4	5.90	1.38	1.34
55	B8	59	A	C5-C4	-5.90	1.34	1.38
1	AA	1102	A	N3-C4	5.90	1.38	1.34
22	BA	233	A	C8-N7	5.90	1.35	1.31
22	BA	2662	A	C5-C4	-5.90	1.34	1.38
22	BA	89	A	N3-C4	5.90	1.38	1.34
22	BA	2468	A	N3-C4	5.90	1.38	1.34
1	AA	873	A	N3-C4	5.90	1.38	1.34
22	BA	1503	A	N3-C4	5.90	1.38	1.34
22	BA	2657	A	N3-C4	5.89	1.38	1.34
1	AA	865	A	N3-C4	5.89	1.38	1.34
22	BA	14	A	C8-N7	5.89	1.35	1.31
1	AA	1269	A	C5-C4	-5.89	1.34	1.38
22	BA	310	A	N3-C4	5.89	1.38	1.34
1	AA	338	A	N3-C4	5.89	1.38	1.34
1	AA	946	A	N3-C4	5.89	1.38	1.34
1	AA	1285	A	N3-C4	5.89	1.38	1.34
1	AA	408	A	C5-C4	-5.88	1.34	1.38
1	AA	539	A	N3-C4	5.88	1.38	1.34
1	AA	129	A	N3-C4	5.88	1.38	1.34
1	AA	1046	A	C5-C4	-5.88	1.34	1.38
22	BA	1175	A	C5-C4	-5.88	1.34	1.38
22	BA	294	A	N3-C4	5.88	1.38	1.34
22	BA	586	A	C8-N7	5.88	1.35	1.31
22	BA	900	A	C5-C4	-5.88	1.34	1.38
22	BA	1916	A	N3-C4	5.88	1.38	1.34
1	AA	814	A	C8-N7	5.88	1.35	1.31
1	AA	1346	A	N3-C4	5.88	1.38	1.34
1	AA	329	A	N3-C4	5.88	1.38	1.34
1	AA	482	A	N3-C4	5.88	1.38	1.34
1	AA	595	A	N3-C4	5.88	1.38	1.34
1	AA	814	A	N3-C4	5.88	1.38	1.34
22	BA	1126	A	C8-N7	5.88	1.35	1.31
22	BA	1268	A	C8-N7	5.88	1.35	1.31
54	B7	8	G	N9-C4	-5.88	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1319	A	N3-C4	5.88	1.38	1.34
22	BA	71	A	N3-C4	5.88	1.38	1.34
1	AA	493	A	N3-C4	5.87	1.38	1.34
1	AA	1363	A	C5-C4	-5.87	1.34	1.38
22	BA	743	A	N3-C4	5.87	1.38	1.34
22	BA	471	A	C8-N7	5.87	1.35	1.31
22	BA	793	A	N3-C4	5.87	1.38	1.34
22	BA	1439	A	N3-C4	5.87	1.38	1.34
22	BA	1635	A	C8-N7	5.87	1.35	1.31
1	AA	1287	A	N3-C4	5.87	1.38	1.34
1	AA	1350	A	C5-C4	-5.87	1.34	1.38
22	BA	49	A	C8-N7	5.87	1.35	1.31
1	AA	546	A	C5-C4	-5.87	1.34	1.38
1	AA	1503	A	C5-C4	-5.87	1.34	1.38
1	AA	759	A	N3-C4	5.87	1.38	1.34
22	BA	2335	A	N7-C5	-5.87	1.35	1.39
22	BA	2411	A	N3-C4	5.87	1.38	1.34
23	BB	34	A	N3-C4	5.87	1.38	1.34
1	AA	923	A	C5-C4	-5.86	1.34	1.38
22	BA	522	A	C8-N7	5.86	1.35	1.31
22	BA	1067	A	C5-C4	-5.86	1.34	1.38
22	BA	1175	A	N3-C4	5.86	1.38	1.34
22	BA	1336	A	N3-C4	5.86	1.38	1.34
22	BA	959	A	N3-C4	5.86	1.38	1.34
22	BA	1866	A	N3-C4	5.86	1.38	1.34
22	BA	251	A	N3-C4	5.86	1.38	1.34
22	BA	255	A	N3-C4	5.86	1.38	1.34
22	BA	345	A	N3-C4	5.86	1.38	1.34
22	BA	2406	A	N3-C4	5.86	1.38	1.34
22	BA	2547	A	N3-C4	5.86	1.38	1.34
22	BA	83	A	N3-C4	5.86	1.38	1.34
22	BA	348	A	N3-C4	5.86	1.38	1.34
22	BA	2560	A	N3-C4	5.86	1.38	1.34
22	BA	2886	A	N3-C4	5.86	1.38	1.34
1	AA	466	A	C5-C4	-5.85	1.34	1.38
1	AA	964	A	N3-C4	5.85	1.38	1.34
1	AA	461	A	C5-C4	-5.85	1.34	1.38
22	BA	1785	A	N3-C4	5.85	1.38	1.34
1	AA	167	A	N3-C4	5.85	1.38	1.34
22	BA	1403	A	N3-C4	5.85	1.38	1.34
1	AA	746	A	C5-C4	-5.85	1.34	1.38
1	AA	1093	A	N3-C4	5.85	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	705	A	N3-C4	5.85	1.38	1.34
22	BA	1010	A	C8-N7	5.85	1.35	1.31
22	BA	1387	A	C5-C4	-5.85	1.34	1.38
22	BA	1598	A	N3-C4	5.85	1.38	1.34
1	AA	825	A	N3-C4	5.85	1.38	1.34
1	AA	914	A	N3-C4	5.85	1.38	1.34
1	AA	977	A	N3-C4	5.85	1.38	1.34
1	AA	1503	A	N3-C4	5.85	1.38	1.34
23	BB	57	A	N3-C4	5.85	1.38	1.34
1	AA	1280	A	C5-C4	-5.85	1.34	1.38
1	AA	1318	A	N3-C4	5.85	1.38	1.34
1	AA	349	A	N3-C4	5.84	1.38	1.34
1	AA	1250	A	N3-C4	5.84	1.38	1.34
1	AA	1271	A	N3-C4	5.84	1.38	1.34
22	BA	1143	A	N3-C4	5.84	1.38	1.34
1	AA	1170	A	C5-C4	-5.84	1.34	1.38
23	BB	15	A	N3-C4	5.84	1.38	1.34
1	AA	493	A	C5-C4	-5.84	1.34	1.38
1	AA	1324	A	C5-C4	-5.84	1.34	1.38
1	AA	909	A	N3-C4	5.84	1.38	1.34
1	AA	546	A	N3-C4	5.84	1.38	1.34
22	BA	1354	A	N7-C5	-5.84	1.35	1.39
22	BA	1889	A	C5-C4	-5.84	1.34	1.38
23	BB	59	A	C5-C4	-5.84	1.34	1.38
1	AA	1055	A	N3-C4	5.83	1.38	1.34
22	BA	861	A	C8-N7	5.83	1.35	1.31
22	BA	2020	A	C8-N7	5.83	1.35	1.31
22	BA	2516	A	C8-N7	5.83	1.35	1.31
1	AA	978	A	C5-C4	-5.83	1.34	1.38
1	AA	1468	A	N3-C4	5.83	1.38	1.34
22	BA	644	A	C8-N7	5.83	1.35	1.31
22	BA	1821	A	C8-N7	5.83	1.35	1.31
1	AA	768	A	C5-C4	-5.83	1.34	1.38
1	AA	1150	A	C5-C4	-5.83	1.34	1.38
22	BA	2199	A	C8-N7	5.83	1.35	1.31
22	BA	1593	A	N3-C4	5.82	1.38	1.34
22	BA	1735	A	N3-C4	5.82	1.38	1.34
22	BA	2662	A	N3-C4	5.82	1.38	1.34
22	BA	330	A	C8-N7	5.82	1.35	1.31
1	AA	309	A	N3-C4	5.82	1.38	1.34
22	BA	52	A	N3-C4	5.82	1.38	1.34
22	BA	1088	A	N3-C4	5.82	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	535	A	N3-C4	5.82	1.38	1.34
1	AA	559	A	C5-C4	-5.82	1.34	1.38
1	AA	621	A	C5-C4	-5.82	1.34	1.38
1	AA	969	A	N3-C4	5.82	1.38	1.34
22	BA	1096	A	C5-C4	-5.82	1.34	1.38
1	AA	792	A	N3-C4	5.82	1.38	1.34
1	AA	1413	A	N3-C4	5.82	1.38	1.34
22	BA	877	A	N3-C4	5.82	1.38	1.34
22	BA	927	A	N3-C4	5.82	1.38	1.34
1	AA	681	A	N3-C4	5.81	1.38	1.34
1	AA	712	A	N3-C4	5.81	1.38	1.34
1	AA	573	A	N3-C4	5.81	1.38	1.34
1	AA	1274	A	C5-C4	-5.81	1.34	1.38
22	BA	2019	A	C8-N7	5.81	1.35	1.31
22	BA	2163	A	C5-C4	-5.81	1.34	1.38
22	BA	2781	A	C8-N7	5.81	1.35	1.31
23	BB	50	A	N3-C4	5.81	1.38	1.34
1	AA	28	A	N3-C4	5.81	1.38	1.34
22	BA	223	A	C8-N7	5.81	1.35	1.31
22	BA	368	A	N3-C4	5.81	1.38	1.34
22	BA	1077	A	N3-C4	5.81	1.38	1.34
22	BA	1672	A	C8-N7	5.81	1.35	1.31
22	BA	1739	A	C5-C4	-5.81	1.34	1.38
22	BA	2352	A	N3-C4	5.81	1.38	1.34
1	AA	179	A	C5-C4	-5.81	1.34	1.38
1	AA	373	A	C5-C4	-5.81	1.34	1.38
22	BA	996	A	C8-N7	5.81	1.35	1.31
1	AA	452	A	C5-C4	-5.81	1.34	1.38
22	BA	637	A	N3-C4	5.81	1.38	1.34
22	BA	2071	A	C5-C4	-5.81	1.34	1.38
22	BA	146	A	N3-C4	5.80	1.38	1.34
22	BA	574	A	C5-C4	-5.80	1.34	1.38
22	BA	1046	A	C5-C4	-5.80	1.34	1.38
22	BA	1544	A	N3-C4	5.80	1.38	1.34
1	AA	192	A	C5-C4	-5.80	1.34	1.38
1	AA	520	A	N3-C4	5.80	1.38	1.34
22	BA	233	A	N3-C4	5.80	1.38	1.34
22	BA	984	A	C8-N7	5.80	1.35	1.31
22	BA	1383	A	N3-C4	5.80	1.38	1.34
22	BA	84	A	N3-C4	5.80	1.38	1.34
22	BA	332	A	N3-C4	5.80	1.38	1.34
22	BA	1700	A	C8-N7	5.80	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1829	A	N3-C4	5.80	1.38	1.34
22	BA	2635	A	N3-C4	5.80	1.38	1.34
22	BA	2893	A	N3-C4	5.80	1.38	1.34
1	AA	50	A	N3-C4	5.80	1.38	1.34
22	BA	1367	A	C8-N7	5.80	1.35	1.31
22	BA	2733	A	N3-C4	5.80	1.38	1.34
22	BA	1969	A	C8-N7	5.80	1.35	1.31
1	AA	602	A	N3-C4	5.80	1.38	1.34
22	BA	2335	A	C5-C4	-5.80	1.34	1.38
1	AA	274	A	N3-C4	5.79	1.38	1.34
1	AA	1111	A	N3-C4	5.79	1.38	1.34
1	AA	223	A	N3-C4	5.79	1.38	1.34
22	BA	751	A	C5-C4	-5.79	1.34	1.38
22	BA	480	A	C8-N7	5.79	1.35	1.31
22	BA	1366	A	C8-N7	5.79	1.35	1.31
22	BA	2879	A	C8-N7	5.79	1.35	1.31
23	BB	101	A	N3-C4	5.79	1.38	1.34
1	AA	663	A	N3-C4	5.79	1.38	1.34
22	BA	2826	A	C8-N7	5.79	1.35	1.31
1	AA	1163	A	C2-N3	5.79	1.38	1.33
1	AA	1229	A	N3-C4	5.79	1.38	1.34
22	BA	514	A	N3-C4	5.79	1.38	1.34
22	BA	2461	A	N3-C4	5.79	1.38	1.34
22	BA	804	A	N3-C4	5.79	1.38	1.34
22	BA	1434	A	C5-C4	-5.79	1.34	1.38
1	AA	33	A	N3-C4	5.79	1.38	1.34
1	AA	1492	A	N3-C4	5.79	1.38	1.34
22	BA	1028	A	N3-C4	5.79	1.38	1.34
22	BA	1505	A	N3-C4	5.79	1.38	1.34
1	AA	533	A	C2-N3	5.78	1.38	1.33
1	AA	782	A	C5-C4	-5.78	1.34	1.38
1	AA	1081	A	N3-C4	5.78	1.38	1.34
1	AA	1375	A	C5-C4	-5.78	1.34	1.38
22	BA	272	A	N3-C4	5.78	1.38	1.34
1	AA	649	A	N3-C4	5.78	1.38	1.34
1	AA	1280	A	N3-C4	5.78	1.38	1.34
22	BA	1001	A	N3-C4	5.78	1.38	1.34
22	BA	1084	A	C5-C4	-5.78	1.34	1.38
22	BA	1553	A	C8-N7	5.78	1.35	1.31
22	BA	2267	A	C8-N7	5.78	1.35	1.31
22	BA	1008	A	C8-N7	5.78	1.35	1.31
22	BA	1070	A	C5-C4	-5.78	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1572	A	C8-N7	5.78	1.35	1.31
22	BA	2033	A	C5-C4	-5.78	1.34	1.38
1	AA	728	A	N3-C4	5.78	1.38	1.34
1	AA	743	A	N3-C4	5.78	1.38	1.34
22	BA	278	A	C5-C4	-5.78	1.34	1.38
22	BA	2726	A	N3-C4	5.78	1.38	1.34
22	BA	2781	A	N3-C4	5.78	1.38	1.34
1	AA	149	A	N3-C4	5.78	1.38	1.34
1	AA	673	A	C5-C4	-5.78	1.34	1.38
1	AA	143	A	N3-C4	5.77	1.38	1.34
1	AA	872	A	N3-C4	5.77	1.38	1.34
22	BA	2173	A	C5-C4	-5.77	1.34	1.38
1	AA	16	A	N3-C4	5.77	1.38	1.34
1	AA	974	A	N3-C4	5.77	1.38	1.34
22	BA	454	A	C5-C4	-5.77	1.34	1.38
22	BA	1028	A	C8-N7	5.77	1.35	1.31
22	BA	2211	A	N3-C4	5.77	1.38	1.34
22	BA	144	A	N3-C4	5.77	1.38	1.34
22	BA	705	A	N7-C5	-5.77	1.35	1.39
22	BA	825	A	N3-C4	5.77	1.38	1.34
22	BA	1535	A	C5-C4	-5.77	1.34	1.38
55	B8	21	A	C5-C4	-5.77	1.34	1.38
1	AA	908	A	N3-C4	5.76	1.38	1.34
1	AA	1042	A	C5-C4	-5.76	1.34	1.38
22	BA	2386	A	N3-C4	5.76	1.38	1.34
23	BB	46	A	C5-C4	-5.76	1.34	1.38
22	BA	861	A	N3-C4	5.76	1.38	1.34
22	BA	2388	A	C8-N7	5.76	1.35	1.31
22	BA	2654	A	C5-C4	-5.76	1.34	1.38
23	BB	94	A	C8-N7	5.76	1.35	1.31
1	AA	648	A	N3-C4	5.76	1.38	1.34
1	AA	906	A	N3-C4	5.76	1.38	1.34
1	AA	1340	A	N3-C4	5.76	1.38	1.34
22	BA	1773	A	C8-N7	5.76	1.35	1.31
23	BB	53	A	N3-C4	5.76	1.38	1.34
55	B8	66	A	C5-C4	-5.76	1.34	1.38
1	AA	1368	A	N3-C4	5.76	1.38	1.34
1	AA	1434	A	N3-C4	5.76	1.38	1.34
22	BA	167	A	N3-C4	5.76	1.38	1.34
1	AA	190	A	C5-C4	-5.76	1.34	1.38
22	BA	460	A	C8-N7	5.76	1.35	1.31
1	AA	119	A	N3-C4	5.75	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	190	A	N7-C5	-5.75	1.35	1.39
22	BA	781	A	C5-C4	-5.75	1.34	1.38
54	B7	9	A	N3-C4	5.75	1.38	1.34
22	BA	432	A	N3-C4	5.75	1.38	1.34
22	BA	825	A	C8-N7	5.75	1.35	1.31
22	BA	1494	A	N3-C4	5.75	1.38	1.34
22	BA	1810	A	N3-C4	5.75	1.38	1.34
1	AA	149	A	C5-C4	-5.75	1.34	1.38
22	BA	1021	A	N3-C4	5.75	1.38	1.34
1	AA	160	A	N3-C4	5.75	1.38	1.34
1	AA	1362	A	N3-C4	5.75	1.38	1.34
22	BA	666	A	C8-N7	5.75	1.35	1.31
22	BA	1127	A	N3-C4	5.75	1.38	1.34
22	BA	2899	A	N3-C4	5.75	1.38	1.34
1	AA	1238	A	N3-C4	5.74	1.38	1.34
22	BA	866	A	N3-C4	5.74	1.38	1.34
22	BA	1086	A	N3-C4	5.74	1.38	1.34
22	BA	1387	A	N3-C4	5.74	1.38	1.34
22	BA	2288	A	C5-C4	-5.74	1.34	1.38
23	BB	104	A	N3-C4	5.74	1.38	1.34
23	BB	108	A	N3-C4	5.74	1.38	1.34
1	AA	1480	A	N3-C4	5.74	1.38	1.34
1	AA	1191	A	C5-C4	-5.74	1.34	1.38
22	BA	943	A	N3-C4	5.74	1.38	1.34
22	BA	1469	A	N3-C4	5.74	1.38	1.34
22	BA	1635	A	N3-C4	5.74	1.38	1.34
1	AA	383	A	C2-N3	5.74	1.38	1.33
1	AA	532	A	C5-C4	-5.74	1.34	1.38
1	AA	1227	A	N3-C4	5.74	1.38	1.34
22	BA	1580	A	N3-C4	5.74	1.38	1.34
1	AA	80	A	C5-C4	-5.73	1.34	1.38
1	AA	196	A	N3-C4	5.73	1.38	1.34
22	BA	374	A	C5-C4	-5.73	1.34	1.38
22	BA	572	A	N3-C4	5.73	1.38	1.34
1	AA	101	A	N3-C4	5.73	1.38	1.34
1	AA	288	A	N3-C4	5.73	1.38	1.34
22	BA	103	A	N3-C4	5.73	1.38	1.34
22	BA	1000	A	N3-C4	5.73	1.38	1.34
22	BA	1080	A	C5-C4	-5.73	1.34	1.38
22	BA	2058	A	C8-N7	5.73	1.35	1.31
22	BA	64	A	N3-C4	5.73	1.38	1.34
22	BA	1241	A	N3-C4	5.73	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1276	A	N3-C4	5.73	1.38	1.34
22	BA	1614	A	C5-C4	-5.73	1.34	1.38
1	AA	1350	A	N3-C4	5.73	1.38	1.34
22	BA	382	A	C8-N7	5.73	1.35	1.31
22	BA	1746	A	N3-C4	5.73	1.38	1.34
1	AA	353	A	N3-C4	5.73	1.38	1.34
1	AA	648	A	C5-C4	-5.73	1.34	1.38
22	BA	2765	A	C8-N7	5.73	1.35	1.31
1	AA	1433	A	N3-C4	5.72	1.38	1.34
22	BA	492	A	C8-N7	5.72	1.35	1.31
22	BA	633	A	C5-C4	-5.72	1.34	1.38
22	BA	1509	A	N3-C4	5.72	1.38	1.34
22	BA	789	A	N3-C4	5.72	1.38	1.34
22	BA	1009	A	N3-C4	5.72	1.38	1.34
22	BA	1705	A	C8-N7	5.72	1.35	1.31
22	BA	2757	A	C5-C4	-5.72	1.34	1.38
22	BA	2758	A	N3-C4	5.72	1.38	1.34
1	AA	1179	A	C5-C4	-5.72	1.34	1.38
22	BA	141	G	C2-N3	5.72	1.37	1.32
1	AA	120	A	N3-C4	5.72	1.38	1.34
22	BA	111	A	N3-C4	5.72	1.38	1.34
22	BA	197	A	N3-C4	5.72	1.38	1.34
22	BA	515	A	C8-N7	5.72	1.35	1.31
1	AA	1236	A	N3-C4	5.72	1.38	1.34
22	BA	244	A	C8-N7	5.72	1.35	1.31
22	BA	749	A	C8-N7	5.72	1.35	1.31
22	BA	899	A	N3-C4	5.72	1.38	1.34
22	BA	1327	A	N3-C4	5.72	1.38	1.34
1	AA	448	A	C5-C4	-5.71	1.34	1.38
1	AA	665	A	N3-C4	5.71	1.38	1.34
1	AA	1287	A	C5-C4	-5.71	1.34	1.38
22	BA	2082	A	N3-C4	5.71	1.38	1.34
1	AA	364	A	N3-C4	5.71	1.38	1.34
1	AA	1468	A	C8-N7	5.71	1.35	1.31
22	BA	127	A	N3-C4	5.71	1.38	1.34
22	BA	2564	A	C8-N7	5.71	1.35	1.31
1	AA	382	A	N3-C4	5.71	1.38	1.34
1	AA	629	A	N3-C4	5.71	1.38	1.34
22	BA	466	A	N3-C4	5.71	1.38	1.34
22	BA	2750	A	N3-C4	5.71	1.38	1.34
22	BA	2134	A	C5-C4	-5.71	1.34	1.38
1	AA	196	A	C5-C4	-5.71	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1819	A	N3-C4	5.71	1.38	1.34
22	BA	1872	A	C5-C4	-5.71	1.34	1.38
22	BA	2352	A	C8-N7	5.71	1.35	1.31
22	BA	2766	A	N3-C4	5.71	1.38	1.34
1	AA	1019	A	N3-C4	5.70	1.38	1.34
1	AA	1082	A	N3-C4	5.70	1.38	1.34
22	BA	1010	A	N3-C4	5.70	1.38	1.34
22	BA	2062	A	N3-C4	5.70	1.38	1.34
22	BA	2284	A	C8-N7	5.70	1.35	1.31
23	BB	45	A	N3-C4	5.70	1.38	1.34
1	AA	441	A	C5-C4	-5.70	1.34	1.38
22	BA	251	A	C5-C4	-5.70	1.34	1.38
1	AA	845	A	C5-C4	-5.70	1.34	1.38
1	AA	1493	A	N3-C4	5.70	1.38	1.34
22	BA	42	A	N3-C4	5.70	1.38	1.34
22	BA	2281	A	N3-C4	5.70	1.38	1.34
1	AA	162	A	C8-N7	5.70	1.35	1.31
1	AA	523	A	N3-C4	5.70	1.38	1.34
22	BA	265	A	N3-C4	5.70	1.38	1.34
22	BA	716	A	N3-C4	5.70	1.38	1.34
22	BA	221	A	N3-C4	5.69	1.38	1.34
22	BA	2270	A	N3-C4	5.69	1.38	1.34
8	AH	96	MET	CB-CG	-5.69	1.33	1.51
22	BA	1664	A	N3-C4	5.69	1.38	1.34
22	BA	2577	A	C5-C4	-5.69	1.34	1.38
22	BA	91	A	N3-C4	5.69	1.38	1.34
22	BA	1785	A	C8-N7	5.69	1.35	1.31
22	BA	2765	A	N3-C4	5.69	1.38	1.34
1	AA	673	A	C2-N3	5.69	1.38	1.33
22	BA	422	A	C5-C4	-5.69	1.34	1.38
1	AA	1171	A	C5-C4	-5.69	1.34	1.38
22	BA	718	A	N3-C4	5.69	1.38	1.34
22	BA	1393	A	N3-C4	5.69	1.38	1.34
22	BA	1655	A	C8-N7	5.69	1.35	1.31
1	AA	1080	A	N3-C4	5.68	1.38	1.34
22	BA	677	A	C8-N7	5.68	1.35	1.31
22	BA	1322	A	C8-N7	5.68	1.35	1.31
22	BA	2572	A	N3-C4	5.68	1.38	1.34
1	AA	1213	A	C5-C4	-5.68	1.34	1.38
22	BA	1392	A	N3-C4	5.68	1.38	1.34
22	BA	2761	A	N3-C4	5.68	1.38	1.34
22	BA	479	A	N3-C4	5.68	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	131	A	N3-C4	5.68	1.38	1.34
22	BA	715	A	N3-C4	5.68	1.38	1.34
22	BA	1155	A	C8-N7	5.68	1.35	1.31
23	BB	99	A	N3-C4	5.68	1.38	1.34
1	AA	1447	A	N3-C4	5.68	1.38	1.34
1	AA	1035	A	C5-C4	-5.67	1.34	1.38
22	BA	1528	A	C8-N7	5.67	1.35	1.31
22	BA	1495	A	C5-C4	-5.67	1.34	1.38
22	BA	1913	A	N3-C4	5.67	1.38	1.34
22	BA	160	A	N3-C4	5.67	1.38	1.34
22	BA	2298	A	N3-C4	5.67	1.38	1.34
23	BB	29	A	N3-C4	5.67	1.38	1.34
22	BA	13	A	N3-C4	5.67	1.38	1.34
22	BA	1853	A	N3-C4	5.67	1.38	1.34
1	AA	959	A	N3-C4	5.67	1.38	1.34
22	BA	56	A	C8-N7	5.67	1.35	1.31
22	BA	497	A	N3-C4	5.67	1.38	1.34
22	BA	909	A	N3-C4	5.67	1.38	1.34
22	BA	1367	A	N3-C4	5.67	1.38	1.34
22	BA	2090	A	C8-N7	5.67	1.35	1.31
1	AA	300	A	C8-N7	5.66	1.35	1.31
1	AA	1170	A	C2-N3	5.66	1.38	1.33
22	BA	190	A	C8-N7	5.66	1.35	1.31
22	BA	996	A	N3-C4	5.66	1.38	1.34
22	BA	2634	A	N3-C4	5.66	1.38	1.34
22	BA	2565	A	C8-N7	5.66	1.35	1.31
1	AA	172	A	N3-C4	5.66	1.38	1.34
22	BA	156	A	N3-C4	5.66	1.38	1.34
22	BA	2191	A	C5-C4	-5.66	1.34	1.38
22	BA	181	A	N3-C4	5.66	1.38	1.34
22	BA	1247	A	N3-C4	5.66	1.38	1.34
1	AA	190	A	C2-N3	5.66	1.38	1.33
22	BA	217	A	N3-C4	5.66	1.38	1.34
1	AA	510	A	N3-C4	5.66	1.38	1.34
22	BA	182	A	N3-C4	5.66	1.38	1.34
22	BA	1966	A	N3-C4	5.65	1.38	1.34
1	AA	1500	A	C5-C4	-5.65	1.34	1.38
22	BA	990	A	C8-N7	5.65	1.35	1.31
22	BA	2077	A	N3-C4	5.65	1.38	1.34
55	B8	73	A	C5-C4	-5.65	1.34	1.38
22	BA	2060	A	N3-C4	5.65	1.38	1.34
22	BA	2169	A	C5-C4	-5.65	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	173	A	N3-C4	5.65	1.38	1.34
22	BA	820	A	N3-C4	5.65	1.38	1.34
1	AA	1117	A	N3-C4	5.65	1.38	1.34
22	BA	742	A	N3-C4	5.65	1.38	1.34
22	BA	2721	A	C5-C4	-5.65	1.34	1.38
1	AA	228	A	N3-C4	5.64	1.38	1.34
22	BA	2705	A	C8-N7	5.64	1.35	1.31
22	BA	342	A	N3-C4	5.64	1.38	1.34
22	BA	415	A	C8-N7	5.64	1.35	1.31
22	BA	608	A	C8-N7	5.64	1.35	1.31
22	BA	1802	A	N3-C4	5.64	1.38	1.34
22	BA	1630	A	N3-C4	5.64	1.38	1.34
22	BA	371	A	N3-C4	5.63	1.38	1.34
22	BA	1597	A	N3-C4	5.63	1.38	1.34
22	BA	2170	A	C5-C4	-5.63	1.34	1.38
22	BA	447	A	N7-C5	-5.63	1.35	1.39
22	BA	1637	A	C8-N7	5.63	1.35	1.31
22	BA	2005	A	N3-C4	5.63	1.38	1.34
22	BA	1264	A	C8-N7	5.63	1.35	1.31
22	BA	1918	A	N3-C4	5.63	1.38	1.34
1	AA	1035	A	C2-N3	5.63	1.38	1.33
22	BA	2776	A	N3-C4	5.63	1.38	1.34
1	AA	574	A	N3-C4	5.63	1.38	1.34
22	BA	1260	A	C8-N7	5.63	1.35	1.31
22	BA	1755	A	N3-C4	5.62	1.38	1.34
22	BA	2199	A	N3-C4	5.62	1.38	1.34
1	AA	116	A	N3-C4	5.62	1.38	1.34
22	BA	1241	A	N7-C5	-5.62	1.35	1.39
22	BA	1603	A	N3-C4	5.62	1.38	1.34
1	AA	889	A	N3-C4	5.62	1.38	1.34
1	AA	983	A	N3-C4	5.62	1.38	1.34
1	AA	1110	A	N3-C4	5.62	1.38	1.34
22	BA	2829	A	N3-C4	5.62	1.38	1.34
22	BA	792	A	C8-N7	5.62	1.35	1.31
22	BA	892	A	C5-C4	-5.62	1.34	1.38
22	BA	256	A	C8-N7	5.62	1.35	1.31
22	BA	2278	A	N3-C4	5.62	1.38	1.34
22	BA	423	A	N3-C4	5.61	1.38	1.34
22	BA	668	A	C8-N7	5.61	1.35	1.31
22	BA	1572	A	N7-C5	-5.61	1.35	1.39
22	BA	1610	A	N3-C4	5.61	1.38	1.34
22	BA	2058	A	N3-C4	5.61	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2227	A	N3-C4	5.61	1.38	1.34
1	AA	236	A	N3-C4	5.61	1.38	1.34
22	BA	2191	A	N3-C4	5.61	1.38	1.34
1	AA	579	A	N3-C4	5.61	1.38	1.34
1	AA	753	A	N3-C4	5.61	1.38	1.34
22	BA	794	A	N3-C4	5.61	1.38	1.34
22	BA	2850	A	N3-C4	5.61	1.38	1.34
22	BA	1608	A	C5-C4	-5.61	1.34	1.38
1	AA	389	A	C2-N3	5.61	1.38	1.33
22	BA	528	A	C8-N7	5.61	1.35	1.31
22	BA	1757	A	C8-N7	5.61	1.35	1.31
22	BA	2328	A	N3-C4	5.61	1.38	1.34
22	BA	1470	A	C5-C4	-5.60	1.34	1.38
1	AA	1	A	C5-C4	-5.60	1.34	1.38
1	AA	782	A	N3-C4	5.60	1.38	1.34
1	AA	1441	A	C2-N3	5.60	1.38	1.33
22	BA	477	A	N3-C4	5.60	1.38	1.34
22	BA	575	A	C8-N7	5.60	1.35	1.31
22	BA	2135	A	C5-C4	-5.60	1.34	1.38
1	AA	482	A	C5-C4	-5.60	1.34	1.38
22	BA	925	A	N3-C4	5.60	1.38	1.34
22	BA	1431	A	C8-N7	5.60	1.35	1.31
22	BA	2810	A	N3-C4	5.60	1.38	1.34
1	AA	77	A	C2-N3	5.60	1.38	1.33
1	AA	563	A	N3-C4	5.60	1.38	1.34
1	AA	1016	A	N3-C4	5.60	1.38	1.34
22	BA	412	A	C8-N7	5.60	1.35	1.31
1	AA	223	A	C5-C4	-5.60	1.34	1.38
1	AA	913	A	N3-C4	5.60	1.38	1.34
22	BA	626	A	N3-C4	5.59	1.38	1.34
22	BA	1668	A	C5-C4	-5.59	1.34	1.38
1	AA	878	A	N3-C4	5.59	1.38	1.34
22	BA	722	A	N3-C4	5.59	1.38	1.34
1	AA	1299	A	N3-C4	5.59	1.38	1.34
22	BA	655	A	N3-C4	5.59	1.38	1.34
22	BA	1057	A	C5-C4	-5.59	1.34	1.38
22	BA	2340	A	N3-C4	5.59	1.38	1.34
1	AA	303	A	N3-C4	5.59	1.38	1.34
22	BA	1969	A	N7-C5	-5.59	1.35	1.39
22	BA	2108	A	C5-C4	-5.59	1.34	1.38
22	BA	2009	A	C8-N7	5.59	1.35	1.31
1	AA	1130	A	N3-C4	5.59	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	101	A	N3-C4	5.59	1.38	1.34
22	BA	2860	A	N3-C4	5.59	1.38	1.34
1	AA	919	A	N3-C4	5.58	1.38	1.34
22	BA	1165	A	N3-C4	5.58	1.38	1.34
22	BA	1213	A	N7-C5	-5.58	1.35	1.39
22	BA	1549	A	N3-C4	5.58	1.38	1.34
22	BA	1551	A	N3-C4	5.58	1.38	1.34
22	BA	1978	A	N3-C4	5.58	1.38	1.34
22	BA	492	A	N7-C5	-5.58	1.35	1.39
22	BA	586	A	C5-C4	-5.58	1.34	1.38
22	BA	1419	A	N3-C4	5.58	1.38	1.34
22	BA	1791	A	C8-N7	5.58	1.35	1.31
22	BA	2738	A	N3-C4	5.58	1.38	1.34
22	BA	443	A	C8-N7	5.58	1.35	1.31
1	AA	1418	A	N3-C4	5.58	1.38	1.34
22	BA	482	A	N7-C5	-5.58	1.35	1.39
22	BA	918	A	N3-C4	5.58	1.38	1.34
22	BA	1654	A	C8-N7	5.58	1.35	1.31
22	BA	2433	A	C8-N7	5.58	1.35	1.31
54	B7	8	G	P-O5'	5.58	1.65	1.59
1	AA	502	A	C2-N3	5.57	1.38	1.33
22	BA	1342	A	N3-C4	5.57	1.38	1.34
22	BA	1579	A	N3-C4	5.57	1.38	1.34
22	BA	1634	A	N3-C4	5.57	1.38	1.34
22	BA	391	A	C8-N7	5.57	1.35	1.31
22	BA	981	A	N3-C4	5.57	1.38	1.34
1	AA	270	A	N3-C4	5.56	1.38	1.34
22	BA	2590	A	N3-C4	5.56	1.38	1.34
1	AA	382	A	C5-C4	-5.56	1.34	1.38
22	BA	2054	A	N3-C4	5.56	1.38	1.34
23	BB	115	A	N3-C4	5.56	1.38	1.34
1	AA	26	A	N3-C4	5.56	1.38	1.34
22	BA	1570	A	C8-N7	5.56	1.35	1.31
22	BA	1572	A	N3-C4	5.56	1.38	1.34
22	BA	1664	A	N7-C5	-5.56	1.35	1.39
1	AA	768	A	N3-C4	5.56	1.38	1.34
22	BA	1095	A	C5-C4	-5.56	1.34	1.38
22	BA	2377	A	N3-C4	5.56	1.38	1.34
1	AA	435	A	C5-C4	-5.56	1.34	1.38
1	AA	1005	A	C5-C4	-5.56	1.34	1.38
1	AA	1456	A	N3-C4	5.56	1.38	1.34
22	BA	1711	A	N3-C4	5.56	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	702	A	N3-C4	5.55	1.38	1.34
1	AA	1357	A	N3-C4	5.55	1.38	1.34
22	BA	693	A	N3-C4	5.55	1.38	1.34
22	BA	2513	A	C8-N7	5.55	1.35	1.31
22	BA	1040	A	N3-C4	5.55	1.38	1.34
55	B8	51	A	N3-C4	5.55	1.38	1.34
22	BA	911	A	C8-N7	5.55	1.35	1.31
1	AA	937	A	N3-C4	5.55	1.38	1.34
22	BA	197	A	N7-C5	-5.55	1.35	1.39
22	BA	471	A	N3-C4	5.55	1.38	1.34
22	BA	753	A	C8-N7	5.55	1.35	1.31
22	BA	1029	A	C8-N7	5.55	1.35	1.31
22	BA	1705	A	N3-C4	5.55	1.38	1.34
1	AA	746	A	C2-N3	5.54	1.38	1.33
22	BA	1969	A	N3-C4	5.54	1.38	1.34
1	AA	300	A	N7-C5	-5.54	1.35	1.39
1	AA	1188	A	N3-C4	5.54	1.38	1.34
22	BA	802	A	N3-C4	5.54	1.38	1.34
1	AA	19	A	N3-C4	5.54	1.38	1.34
22	BA	457	A	N3-C4	5.54	1.38	1.34
22	BA	1032	A	N3-C4	5.54	1.38	1.34
22	BA	1652	A	N7-C5	-5.54	1.35	1.39
22	BA	1970	A	N3-C4	5.54	1.38	1.34
22	BA	730	A	N7-C5	-5.54	1.35	1.39
22	BA	1134	A	N3-C4	5.54	1.38	1.34
22	BA	2126	A	C5-C4	-5.54	1.34	1.38
22	BA	1794	A	N3-C4	5.54	1.38	1.34
22	BA	1689	A	N3-C4	5.54	1.38	1.34
22	BA	2005	A	C8-N7	5.54	1.35	1.31
1	AA	60	A	N3-C4	5.53	1.38	1.34
1	AA	1377	A	N3-C4	5.53	1.38	1.34
22	BA	10	A	N3-C4	5.53	1.38	1.34
22	BA	574	A	N3-C4	5.53	1.38	1.34
22	BA	1871	A	N3-C4	5.53	1.38	1.34
22	BA	2448	A	N3-C4	5.53	1.38	1.34
22	BA	2598	A	N3-C4	5.53	1.38	1.34
22	BA	631	A	C8-N7	5.53	1.35	1.31
1	AA	44	A	N3-C4	5.53	1.38	1.34
22	BA	324	A	N3-C4	5.53	1.38	1.34
22	BA	1668	A	N7-C5	-5.53	1.35	1.39
22	BA	1890	A	N3-C4	5.53	1.38	1.34
22	BA	721	A	N3-C4	5.53	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1932	A	N3-C4	5.53	1.38	1.34
1	AA	431	A	N3-C4	5.53	1.38	1.34
22	BA	207	A	N3-C4	5.53	1.38	1.34
22	BA	401	A	C8-N7	5.53	1.35	1.31
22	BA	1009	A	C8-N7	5.53	1.35	1.31
22	BA	1098	A	C2-N3	5.53	1.38	1.33
22	BA	1308	A	N3-C4	5.53	1.38	1.34
22	BA	1717	A	N3-C4	5.53	1.38	1.34
22	BA	1899	A	C8-N7	5.53	1.35	1.31
22	BA	95	A	N3-C4	5.52	1.38	1.34
22	BA	1194	A	N3-C4	5.52	1.38	1.34
22	BA	1981	A	N3-C4	5.52	1.38	1.34
1	AA	622	A	N3-C4	5.52	1.38	1.34
1	AA	780	A	N3-C4	5.52	1.38	1.34
22	BA	241	A	N3-C4	5.52	1.38	1.34
1	AA	1534	A	C5-C4	-5.52	1.34	1.38
22	BA	447	A	C8-N7	5.52	1.35	1.31
22	BA	483	A	N3-C4	5.52	1.38	1.34
22	BA	2749	A	C5-C4	-5.52	1.34	1.38
55	B8	14	A	C5-C4	-5.52	1.34	1.38
22	BA	2366	A	N3-C4	5.52	1.38	1.34
1	AA	3	A	N3-C4	5.51	1.38	1.34
1	AA	10	A	N3-C4	5.51	1.38	1.34
1	AA	509	A	N3-C4	5.51	1.38	1.34
22	BA	52	A	C8-N7	5.51	1.35	1.31
1	AA	747	A	C5-C4	-5.51	1.34	1.38
22	BA	2721	A	C8-N7	5.51	1.35	1.31
1	AA	131	A	N3-C4	5.51	1.38	1.34
1	AA	366	A	N3-C4	5.51	1.38	1.34
22	BA	309	A	N3-C4	5.51	1.38	1.34
22	BA	1039	A	N3-C4	5.51	1.38	1.34
22	BA	2883	A	C8-N7	5.51	1.35	1.31
22	BA	2077	A	N7-C5	-5.51	1.35	1.39
22	BA	2154	A	C2-N3	5.51	1.38	1.33
1	AA	968	A	N3-C4	5.51	1.38	1.34
1	AA	1430	A	N3-C4	5.51	1.38	1.34
22	BA	590	A	N3-C4	5.51	1.38	1.34
22	BA	972	A	C8-N7	5.50	1.35	1.31
1	AA	452	A	N3-C4	5.50	1.38	1.34
22	BA	1054	A	C2-N3	5.50	1.38	1.33
22	BA	1359	A	N3-C4	5.50	1.38	1.34
22	BA	917	A	N3-C4	5.50	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	777	A	N3-C4	5.50	1.38	1.34
22	BA	599	A	C8-N7	5.50	1.35	1.31
22	BA	1889	A	N3-C4	5.50	1.38	1.34
22	BA	1654	A	N3-C4	5.50	1.38	1.34
22	BA	2820	A	N3-C4	5.50	1.38	1.34
1	AA	55	A	C2-N3	5.50	1.38	1.33
22	BA	819	A	N3-C4	5.50	1.38	1.34
22	BA	528	A	N3-C4	5.49	1.38	1.34
22	BA	947	A	N3-C4	5.49	1.38	1.34
22	BA	2459	A	C8-N7	5.49	1.35	1.31
22	BA	2273	A	C8-N7	5.49	1.35	1.31
1	AA	478	A	C5-C4	-5.49	1.34	1.38
22	BA	1608	A	N3-C4	5.49	1.38	1.34
22	BA	1912	A	N3-C4	5.49	1.38	1.34
1	AA	860	A	N3-C4	5.49	1.38	1.34
22	BA	2088	A	N3-C4	5.49	1.38	1.34
23	BB	78	A	N3-C4	5.49	1.38	1.34
22	BA	1048	A	C5-C4	-5.49	1.34	1.38
1	AA	860	A	C5-C4	-5.49	1.34	1.38
1	AA	1219	A	C2-N3	5.49	1.38	1.33
22	BA	1096	A	C2-N3	5.49	1.38	1.33
1	AA	1499	A	N3-C4	5.48	1.38	1.34
22	BA	1008	A	N3-C4	5.48	1.38	1.34
22	BA	1678	A	C8-N7	5.48	1.35	1.31
22	BA	256	A	N3-C4	5.48	1.38	1.34
22	BA	2170	A	C2-N3	5.48	1.38	1.33
1	AA	900	A	N3-C4	5.48	1.38	1.34
22	BA	1952	A	C8-N7	5.48	1.35	1.31
22	BA	1936	A	C2-N3	5.48	1.38	1.33
1	AA	1067	A	N3-C4	5.47	1.38	1.34
22	BA	1265	A	N7-C5	-5.47	1.35	1.39
22	BA	2541	A	C8-N7	5.47	1.35	1.31
22	BA	161	A	N3-C4	5.47	1.38	1.34
22	BA	764	A	N3-C4	5.47	1.38	1.34
22	BA	1650	A	N3-C4	5.47	1.38	1.34
22	BA	1854	A	N3-C4	5.47	1.38	1.34
22	BA	2900	A	N3-C4	5.47	1.38	1.34
22	BA	244	A	N3-C4	5.47	1.38	1.34
1	AA	794	A	N3-C4	5.47	1.38	1.34
22	BA	505	A	N7-C5	-5.47	1.35	1.39
22	BA	1020	A	N3-C4	5.47	1.38	1.34
22	BA	1262	A	C8-N7	5.47	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1213	A	N3-C4	5.47	1.38	1.34
22	BA	1143	A	C8-N7	5.47	1.35	1.31
22	BA	2225	A	N3-C4	5.47	1.38	1.34
22	BA	2826	A	N3-C4	5.47	1.38	1.34
55	B8	69	A	N3-C4	5.47	1.38	1.34
1	AA	1465	A	N3-C4	5.46	1.38	1.34
22	BA	126	A	C8-N7	5.46	1.35	1.31
22	BA	401	A	N3-C4	5.46	1.38	1.34
22	BA	1847	A	N3-C4	5.46	1.38	1.34
22	BA	2070	A	N3-C4	5.46	1.38	1.34
22	BA	2453	A	C8-N7	5.46	1.35	1.31
1	AA	790	A	N3-C4	5.46	1.38	1.34
22	BA	2052	A	N3-C4	5.46	1.38	1.34
22	BA	1080	A	C2-N3	5.46	1.38	1.33
22	BA	2247	A	C8-N7	5.46	1.35	1.31
22	BA	556	A	C8-N7	5.46	1.35	1.31
22	BA	2176	A	C5-C4	-5.46	1.34	1.38
22	BA	2274	A	N7-C5	-5.46	1.35	1.39
1	AA	66	A	N3-C4	5.46	1.38	1.34
1	AA	1130	A	C5-C4	-5.46	1.34	1.38
22	BA	125	A	N3-C4	5.46	1.38	1.34
22	BA	2241	A	N3-C4	5.46	1.38	1.34
22	BA	2322	A	N3-C4	5.46	1.38	1.34
22	BA	2577	A	N7-C5	-5.46	1.35	1.39
22	BA	2809	A	N3-C4	5.46	1.38	1.34
1	AA	1408	A	N3-C4	5.46	1.38	1.34
22	BA	49	A	N7-C5	-5.46	1.35	1.39
22	BA	1129	A	C8-N7	5.46	1.35	1.31
1	AA	807	A	N3-C4	5.45	1.38	1.34
22	BA	988	A	C8-N7	5.45	1.35	1.31
22	BA	988	A	N3-C4	5.45	1.38	1.34
22	BA	1784	A	C8-N7	5.45	1.35	1.31
22	BA	1354	A	N3-C4	5.45	1.38	1.34
22	BA	2635	A	C8-N7	5.45	1.35	1.31
22	BA	2740	A	N3-C4	5.45	1.38	1.34
22	BA	983	A	C8-N7	5.45	1.35	1.31
22	BA	2267	A	N3-C4	5.45	1.38	1.34
23	BB	59	A	N1-C2	5.45	1.39	1.34
22	BA	614	A	N3-C4	5.45	1.38	1.34
22	BA	429	A	N3-C4	5.44	1.38	1.34
22	BA	844	A	N3-C4	5.44	1.38	1.34
22	BA	2314	A	N3-C4	5.44	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1431	A	N3-C4	5.44	1.38	1.34
22	BA	592	A	N3-C4	5.44	1.38	1.34
22	BA	910	A	C8-N7	5.44	1.35	1.31
22	BA	1147	A	N3-C4	5.44	1.38	1.34
22	BA	2632	A	N3-C4	5.44	1.38	1.34
22	BA	819	A	N7-C5	-5.44	1.35	1.39
22	BA	2439	A	N3-C4	5.44	1.38	1.34
22	BA	402	A	N3-C4	5.44	1.38	1.34
22	BA	1010	A	C5-C4	-5.44	1.34	1.38
22	BA	2764	A	N3-C4	5.44	1.38	1.34
22	BA	1801	A	N3-C4	5.43	1.38	1.34
22	BA	2778	A	N3-C4	5.43	1.38	1.34
55	B8	6	A	N3-C4	5.43	1.38	1.34
1	AA	1507	A	N3-C4	5.43	1.38	1.34
22	BA	541	A	N3-C4	5.43	1.38	1.34
1	AA	383	A	C8-N7	5.43	1.35	1.31
22	BA	1373	A	N3-C4	5.43	1.38	1.34
22	BA	2042	A	N3-C4	5.43	1.38	1.34
1	AA	363	A	N3-C4	5.43	1.38	1.34
22	BA	936	A	N3-C4	5.43	1.38	1.34
22	BA	1571	A	C8-N7	5.43	1.35	1.31
1	AA	151	A	N3-C4	5.43	1.38	1.34
1	AA	199	A	C2-N3	5.43	1.38	1.33
22	BA	983	A	N7-C5	-5.43	1.35	1.39
22	BA	2037	A	C8-N7	5.43	1.35	1.31
1	AA	787	A	N3-C4	5.42	1.38	1.34
1	AA	415	A	C5-C4	-5.42	1.34	1.38
1	AA	1176	A	N3-C4	5.42	1.38	1.34
22	BA	1665	A	C8-N7	5.42	1.35	1.31
22	BA	1021	A	N7-C5	-5.42	1.35	1.39
22	BA	2095	A	N3-C4	5.42	1.38	1.34
1	AA	975	A	N3-C4	5.42	1.38	1.34
22	BA	1103	A	C2-N3	5.42	1.38	1.33
22	BA	2378	A	N3-C4	5.42	1.38	1.34
1	AA	397	A	C2-N3	5.41	1.38	1.33
1	AA	640	A	C2-N3	5.41	1.38	1.33
1	AA	1101	A	N3-C4	5.41	1.38	1.34
22	BA	191	A	C8-N7	5.41	1.35	1.31
22	BA	311	A	N3-C4	5.41	1.38	1.34
22	BA	1698	A	N3-C4	5.41	1.38	1.34
1	AA	383	A	C5-C4	-5.41	1.34	1.38
22	BA	2369	A	N3-C4	5.41	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	526	A	N3-C4	5.41	1.38	1.34
22	BA	2412	A	C8-N7	5.41	1.35	1.31
22	BA	2297	A	N3-C4	5.41	1.38	1.34
22	BA	19	A	N3-C4	5.40	1.38	1.34
1	AA	1261	A	C2-N3	5.40	1.38	1.33
22	BA	1759	A	C8-N7	5.40	1.35	1.31
22	BA	2450	A	C5-C4	-5.40	1.34	1.38
22	BA	2497	A	N7-C5	-5.40	1.36	1.39
22	BA	973	A	N3-C4	5.40	1.38	1.34
22	BA	2873	A	N3-C4	5.40	1.38	1.34
1	AA	162	A	C2-N3	5.40	1.38	1.33
22	BA	172	A	N3-C4	5.40	1.38	1.34
22	BA	1635	A	N7-C5	-5.40	1.36	1.39
1	AA	459	A	C2-N3	5.39	1.38	1.33
22	BA	1321	A	N3-C4	5.39	1.38	1.34
22	BA	1899	A	N7-C5	-5.39	1.36	1.39
1	AA	320	A	N3-C4	5.39	1.38	1.34
22	BA	2660	A	N3-C4	5.39	1.38	1.34
1	AA	784	A	N3-C4	5.39	1.38	1.34
1	AA	321	A	N3-C4	5.39	1.38	1.34
22	BA	2126	A	C2-N3	5.39	1.38	1.33
22	BA	19	A	C8-N7	5.39	1.35	1.31
22	BA	482	A	N3-C4	5.39	1.38	1.34
22	BA	2184	A	C2-N3	5.39	1.38	1.33
1	AA	60	A	C2-N3	5.38	1.38	1.33
22	BA	1088	A	C2-N3	5.38	1.38	1.33
22	BA	1872	A	C2-N3	5.38	1.38	1.33
22	BA	2333	A	N3-C4	5.38	1.38	1.34
22	BA	447	A	N3-C4	5.38	1.38	1.34
22	BA	792	A	N7-C5	-5.38	1.36	1.39
22	BA	2015	A	C8-N7	5.38	1.35	1.31
22	BA	2534	A	N3-C4	5.38	1.38	1.34
1	AA	382	A	C2-N3	5.38	1.38	1.33
1	AA	1508	A	N3-C4	5.38	1.38	1.34
22	BA	2469	A	N3-C4	5.38	1.38	1.34
22	BA	391	A	N3-C4	5.38	1.38	1.34
22	BA	439	A	N3-C4	5.38	1.38	1.34
23	BB	109	A	N3-C4	5.38	1.38	1.34
22	BA	1640	A	N3-C4	5.38	1.38	1.34
22	BA	1286	A	N3-C4	5.37	1.38	1.34
22	BA	1762	A	N3-C4	5.37	1.38	1.34
22	BA	2051	A	N7-C5	-5.37	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	933	A	N3-C4	5.37	1.38	1.34
22	BA	2872	A	C5-C4	-5.37	1.34	1.38
22	BA	863	A	N3-C4	5.37	1.38	1.34
22	BA	1650	A	C8-N7	5.37	1.35	1.31
22	BA	2823	A	C8-N7	5.37	1.35	1.31
1	AA	81	A	C5-C4	-5.37	1.34	1.38
1	AA	263	A	N3-C4	5.37	1.38	1.34
22	BA	56	A	N3-C4	5.37	1.38	1.34
22	BA	1552	A	N3-C4	5.37	1.38	1.34
22	BA	2278	A	C8-N7	5.37	1.35	1.31
1	AA	101	A	C2-N3	5.36	1.38	1.33
1	AA	238	A	N3-C4	5.36	1.38	1.34
22	BA	609	A	N3-C4	5.36	1.38	1.34
22	BA	821	A	C8-N7	5.36	1.35	1.31
22	BA	374	A	N3-C4	5.36	1.38	1.34
22	BA	685	A	C8-N7	5.36	1.35	1.31
22	BA	1301	A	N3-C4	5.36	1.38	1.34
22	BA	1669	A	N7-C5	-5.36	1.36	1.39
22	BA	412	A	N3-C4	5.36	1.38	1.34
1	AA	195	A	N3-C4	5.36	1.38	1.34
1	AA	8	A	N3-C4	5.36	1.38	1.34
1	AA	300	A	C2-N3	5.36	1.38	1.33
22	BA	300	A	N3-C4	5.36	1.38	1.34
22	BA	470	A	N7-C5	-5.36	1.36	1.39
1	AA	1171	A	C2-N3	5.35	1.38	1.33
22	BA	453	A	N3-C4	5.35	1.38	1.34
1	AA	1418	A	C8-N7	5.35	1.35	1.31
22	BA	2589	A	C8-N7	5.35	1.35	1.31
22	BA	2873	A	N7-C5	-5.35	1.36	1.39
22	BA	1722	A	C2-N3	5.35	1.38	1.33
22	BA	2736	A	N3-C4	5.35	1.38	1.34
1	AA	642	A	N3-C4	5.35	1.38	1.34
22	BA	222	A	N3-C4	5.35	1.38	1.34
22	BA	505	A	N3-C4	5.35	1.38	1.34
1	AA	901	A	N3-C4	5.34	1.38	1.34
1	AA	1000	A	C2-N3	5.34	1.38	1.33
22	BA	572	A	C8-N7	5.34	1.35	1.31
22	BA	1784	A	N3-C4	5.34	1.38	1.34
1	AA	371	A	N3-C4	5.34	1.38	1.34
1	AA	1152	A	C2-N3	5.34	1.38	1.33
22	BA	1302	A	N3-C4	5.34	1.38	1.34
22	BA	2412	A	N3-C4	5.34	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2450	A	N3-C4	5.34	1.38	1.34
22	BA	430	A	N3-C4	5.34	1.38	1.34
22	BA	155	A	N3-C4	5.34	1.38	1.34
22	BA	2247	A	N3-C4	5.34	1.38	1.34
22	BA	2705	A	N3-C4	5.34	1.38	1.34
1	AA	716	A	N3-C4	5.34	1.38	1.34
1	AA	1513	A	N3-C4	5.34	1.38	1.34
22	BA	1253	A	N3-C4	5.34	1.38	1.34
22	BA	2071	A	N3-C4	5.34	1.38	1.34
22	BA	2800	A	N3-C4	5.34	1.38	1.34
22	BA	2205	A	N3-C4	5.33	1.38	1.34
22	BA	538	A	N3-C4	5.33	1.38	1.34
22	BA	1998	A	N3-C4	5.33	1.38	1.34
22	BA	2433	A	N3-C4	5.33	1.38	1.34
55	B8	21	A	N3-C4	5.33	1.38	1.34
1	AA	1257	A	C2-N3	5.33	1.38	1.33
1	AA	389	A	C5-C4	-5.33	1.35	1.38
1	AA	994	A	C2-N3	5.33	1.38	1.33
22	BA	502	A	N3-C4	5.33	1.38	1.34
22	BA	547	A	C2-N3	5.33	1.38	1.33
22	BA	1641	A	N3-C4	5.33	1.38	1.34
22	BA	670	A	C8-N7	5.33	1.35	1.31
22	BA	1205	A	N3-C4	5.33	1.38	1.34
22	BA	104	A	N3-C4	5.32	1.38	1.34
22	BA	362	A	C2-N3	5.32	1.38	1.33
22	BA	404	A	N3-C4	5.32	1.38	1.34
22	BA	1504	A	N3-C4	5.32	1.38	1.34
22	BA	1553	A	N7-C5	-5.32	1.36	1.39
1	AA	729	A	N3-C4	5.32	1.38	1.34
22	BA	49	A	N3-C4	5.32	1.38	1.34
22	BA	1757	A	N3-C4	5.32	1.38	1.34
22	BA	1773	A	N7-C5	-5.32	1.36	1.39
1	AA	53	A	C2-N3	5.32	1.38	1.33
1	AA	1055	A	C2-N3	5.32	1.38	1.33
22	BA	613	A	C2-N3	5.32	1.38	1.33
22	BA	1156	A	C8-N7	5.32	1.35	1.31
1	AA	864	A	N3-C4	5.32	1.38	1.34
22	BA	532	A	N3-C4	5.32	1.38	1.34
22	BA	1244	A	C8-N7	5.32	1.35	1.31
22	BA	1802	A	C8-N7	5.31	1.35	1.31
22	BA	1821	A	N3-C4	5.31	1.38	1.34
22	BA	1847	A	C5-C4	-5.31	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	431	A	C5-C4	-5.31	1.35	1.38
1	AA	1004	A	C2-N3	5.31	1.38	1.33
22	BA	920	A	N3-C4	5.31	1.38	1.34
22	BA	2392	A	N3-C4	5.31	1.38	1.34
22	BA	428	A	N3-C4	5.31	1.38	1.34
22	BA	1272	A	N3-C4	5.31	1.38	1.34
1	AA	270	A	C2-N3	5.31	1.38	1.33
1	AA	532	A	C2-N3	5.31	1.38	1.33
1	AA	1	A	C2-N3	5.30	1.38	1.33
1	AA	1188	A	C2-N3	5.30	1.38	1.33
22	BA	751	A	C8-N7	5.30	1.35	1.31
22	BA	1805	A	N3-C4	5.30	1.38	1.34
22	BA	2176	A	C2-N3	5.30	1.38	1.33
55	B8	58	A	N3-C4	5.30	1.38	1.34
22	BA	735	A	N3-C4	5.30	1.38	1.34
22	BA	1014	A	N3-C4	5.30	1.38	1.34
22	BA	1802	A	N7-C5	-5.30	1.36	1.39
1	AA	978	A	N3-C4	5.30	1.38	1.34
22	BA	654	A	C2-N3	5.30	1.38	1.33
22	BA	1275	A	N3-C4	5.30	1.38	1.34
22	BA	983	A	N3-C4	5.30	1.38	1.34
1	AA	415	A	C2-N3	5.30	1.38	1.33
1	AA	1167	A	C2-N3	5.30	1.38	1.33
1	AA	1227	A	C5-C4	-5.30	1.35	1.38
22	BA	905	A	N3-C4	5.30	1.38	1.34
22	BA	2147	A	C5-C4	-5.29	1.35	1.38
22	BA	1095	A	C2-N3	5.29	1.38	1.33
22	BA	2270	A	N7-C5	-5.29	1.36	1.39
22	BA	1204	A	N3-C4	5.29	1.38	1.34
1	AA	1151	A	C2-N3	5.29	1.38	1.33
22	BA	203	A	N3-C4	5.29	1.38	1.34
22	BA	621	A	N3-C4	5.29	1.38	1.34
22	BA	1502	A	N3-C4	5.29	1.38	1.34
22	BA	1525	A	N3-C4	5.29	1.38	1.34
1	AA	1197	A	C2-N3	5.29	1.38	1.33
1	AA	1271	A	C2-N3	5.29	1.38	1.33
22	BA	44	A	N3-C4	5.29	1.38	1.34
22	BA	199	A	N3-C4	5.29	1.38	1.34
22	BA	218	A	N3-C4	5.29	1.38	1.34
22	BA	1470	A	C2-N3	5.29	1.38	1.33
22	BA	1637	A	N3-C4	5.29	1.38	1.34
22	BA	739	A	N3-C4	5.29	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1569	A	N3-C4	5.29	1.38	1.34
22	BA	1603	A	C8-N7	5.29	1.35	1.31
22	BA	2003	A	N3-C4	5.29	1.38	1.34
22	BA	1269	A	C8-N7	5.28	1.35	1.31
1	AA	498	A	N1-C2	5.28	1.39	1.34
1	AA	1246	A	C2-N3	5.28	1.38	1.33
22	BA	1264	A	N7-C5	-5.28	1.36	1.39
22	BA	2212	A	N3-C4	5.28	1.38	1.34
1	AA	520	A	C5-C4	-5.28	1.35	1.38
22	BA	522	A	N3-C4	5.28	1.38	1.34
1	AA	715	A	N3-C4	5.28	1.38	1.34
1	AA	1446	A	C5-C4	-5.28	1.35	1.38
22	BA	794	A	C8-N7	5.28	1.35	1.31
1	AA	174	A	C2-N3	5.28	1.38	1.33
22	BA	514	A	C8-N7	5.28	1.35	1.31
22	BA	586	A	N7-C5	-5.28	1.36	1.39
22	BA	972	A	N3-C4	5.28	1.38	1.34
22	BA	119	A	N3-C4	5.28	1.38	1.34
22	BA	1676	A	C8-N7	5.28	1.35	1.31
22	BA	2358	A	C8-N7	5.28	1.35	1.31
22	BA	1226	A	C8-N7	5.27	1.35	1.31
22	BA	2158	A	C2-N3	5.27	1.38	1.33
1	AA	32	A	C2-N3	5.27	1.38	1.33
22	BA	415	A	N3-C4	5.27	1.38	1.34
22	BA	1285	A	N3-C4	5.27	1.38	1.34
22	BA	1901	A	N3-C4	5.27	1.38	1.34
22	BA	2459	A	N3-C4	5.27	1.38	1.34
22	BA	28	A	C8-N7	5.26	1.35	1.31
22	BA	750	A	C8-N7	5.26	1.35	1.31
22	BA	2346	A	N3-C4	5.26	1.38	1.34
22	BA	2614	A	N3-C4	5.26	1.38	1.34
1	AA	1176	A	C2-N3	5.26	1.38	1.33
22	BA	1591	A	C2-N3	5.26	1.38	1.33
22	BA	1677	A	N7-C5	-5.26	1.36	1.39
22	BA	2727	A	N3-C4	5.26	1.38	1.34
1	AA	712	A	C2-N3	5.26	1.38	1.33
1	AA	1502	A	N3-C4	5.26	1.38	1.34
22	BA	675	A	C8-N7	5.26	1.35	1.31
22	BA	1596	A	N3-C4	5.26	1.38	1.34
22	BA	2266	A	N3-C4	5.26	1.38	1.34
22	BA	2366	A	C8-N7	5.26	1.35	1.31
22	BA	2679	A	N3-C4	5.26	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	B8	76	A	C8-N7	5.26	1.35	1.31
22	BA	2013	A	N7-C5	-5.25	1.36	1.39
22	BA	2821	A	N3-C4	5.25	1.38	1.34
21	AU	2	PRO	CG-CD	-5.25	1.33	1.50
22	BA	706	A	N3-C4	5.25	1.38	1.34
1	AA	78	A	C2-N3	5.24	1.38	1.33
1	AA	1350	A	C2-N3	5.24	1.38	1.33
22	BA	2757	A	C2-N3	5.24	1.38	1.33
22	BA	1431	A	N3-C4	5.24	1.38	1.34
22	BA	2169	A	C2-N3	5.24	1.38	1.33
1	AA	408	A	C2-N3	5.24	1.38	1.33
1	AA	819	A	N3-C4	5.24	1.38	1.34
22	BA	320	A	N3-C4	5.24	1.38	1.34
22	BA	226	A	N3-C4	5.24	1.38	1.34
22	BA	833	A	N3-C4	5.24	1.38	1.34
22	BA	1103	A	C5-C4	-5.24	1.35	1.38
1	AA	162	A	N7-C5	-5.24	1.36	1.39
22	BA	643	A	N3-C4	5.24	1.38	1.34
22	BA	676	A	N3-C4	5.24	1.38	1.34
1	AA	1248	A	C2-N3	5.23	1.38	1.33
1	AA	1299	A	C2-N3	5.23	1.38	1.33
1	AA	189	A	C2-N3	5.23	1.38	1.33
1	AA	487	A	C2-N3	5.23	1.38	1.33
1	AA	958	A	N3-C4	5.23	1.38	1.34
1	AA	938	A	C2-N3	5.23	1.38	1.33
22	BA	1070	A	C2-N3	5.23	1.38	1.33
22	BA	1189	A	C8-N7	5.23	1.35	1.31
22	BA	1535	A	C2-N3	5.23	1.38	1.33
1	AA	155	A	C2-N3	5.23	1.38	1.33
22	BA	2873	A	C8-N7	5.23	1.35	1.31
1	AA	7	A	N3-C4	5.22	1.38	1.34
1	AA	1275	A	C2-N3	5.22	1.38	1.33
1	AA	1339	A	N3-C4	5.22	1.38	1.34
22	BA	1241	A	C8-N7	5.22	1.35	1.31
22	BA	1919	A	N3-C4	5.22	1.38	1.34
22	BA	2009	A	N3-C4	5.22	1.38	1.34
1	AA	1191	A	C2-N3	5.22	1.38	1.33
1	AA	1360	A	N3-C4	5.22	1.38	1.34
22	BA	1029	A	N7-C5	-5.22	1.36	1.39
22	BA	2094	A	C2-N3	5.22	1.38	1.33
22	BA	2670	A	N3-C4	5.22	1.38	1.34
22	BA	661	A	N3-C4	5.22	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1609	A	N3-C4	5.22	1.38	1.34
22	BA	101	A	C2-N3	5.22	1.38	1.33
22	BA	322	A	N3-C4	5.22	1.38	1.34
22	BA	1057	A	C2-N3	5.22	1.38	1.33
22	BA	2163	A	C2-N3	5.22	1.38	1.33
22	BA	482	A	C8-N7	5.22	1.35	1.31
22	BA	1230	A	N3-C4	5.22	1.38	1.34
22	BA	2675	A	C8-N7	5.22	1.35	1.31
1	AA	892	A	N3-C4	5.21	1.38	1.34
22	BA	1786	A	N3-C4	5.21	1.38	1.34
1	AA	1012	A	C2-N3	5.21	1.38	1.33
1	AA	468	A	C2-N3	5.21	1.38	1.33
22	BA	191	A	N3-C4	5.21	1.38	1.34
22	BA	917	A	C8-N7	5.21	1.35	1.31
22	BA	2741	A	N7-C5	-5.21	1.36	1.39
22	BA	820	A	C8-N7	5.21	1.35	1.31
22	BA	2837	A	N3-C4	5.21	1.38	1.34
1	AA	600	A	N3-C4	5.21	1.38	1.34
1	AA	1483	A	C8-N7	5.20	1.35	1.31
22	BA	1144	A	N3-C4	5.20	1.38	1.34
22	BA	2471	A	N3-C4	5.20	1.38	1.34
22	BA	685	A	N3-C4	5.20	1.38	1.34
22	BA	2173	A	C2-N3	5.20	1.38	1.33
1	AA	553	A	C2-N3	5.20	1.38	1.33
1	AA	607	A	N3-C4	5.20	1.38	1.34
1	AA	747	A	C2-N3	5.20	1.38	1.33
1	AA	98	A	C2-N3	5.20	1.38	1.33
1	AA	460	A	C2-N3	5.20	1.38	1.33
1	AA	602	A	C2-N3	5.20	1.38	1.33
22	BA	735	A	N7-C5	-5.20	1.36	1.39
22	BA	1515	A	N3-C4	5.20	1.38	1.34
22	BA	1570	A	N3-C4	5.20	1.38	1.34
22	BA	1641	A	N7-C5	-5.20	1.36	1.39
22	BA	1977	A	N3-C4	5.20	1.38	1.34
22	BA	2706	A	N3-C4	5.20	1.38	1.34
22	BA	802	A	C8-N7	5.20	1.35	1.31
22	BA	2476	A	N3-C4	5.20	1.38	1.34
22	BA	2037	A	N3-C4	5.20	1.38	1.34
1	AA	459	A	C5-C4	-5.19	1.35	1.38
1	AA	1483	A	N7-C5	-5.19	1.36	1.39
22	BA	1786	A	C8-N7	5.19	1.35	1.31
22	BA	2097	A	C2-N3	5.19	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	223	A	C2-N3	5.19	1.38	1.33
1	AA	915	A	N3-C4	5.19	1.38	1.34
22	BA	532	A	C8-N7	5.19	1.35	1.31
22	BA	1090	A	C2-N3	5.19	1.38	1.33
23	BB	58	A	N3-C4	5.19	1.38	1.34
22	BA	1264	A	N3-C4	5.19	1.38	1.34
23	BB	46	A	N3-C4	5.19	1.38	1.34
22	BA	2090	A	N3-C4	5.19	1.38	1.34
1	AA	816	A	N3-C4	5.19	1.38	1.34
22	BA	730	A	C8-N7	5.19	1.35	1.31
1	AA	1288	A	C2-N3	5.18	1.38	1.33
22	BA	1254	A	N3-C4	5.18	1.38	1.34
1	AA	1105	A	C2-N3	5.18	1.38	1.33
22	BA	975	A	C5-C4	-5.18	1.35	1.38
22	BA	1073	A	C2-N3	5.18	1.38	1.33
22	BA	1089	A	C2-N3	5.18	1.38	1.33
22	BA	1262	A	N7-C5	-5.18	1.36	1.39
22	BA	2530	A	N3-C4	5.18	1.38	1.34
1	AA	802	A	N3-C4	5.18	1.38	1.34
22	BA	299	A	N3-C4	5.18	1.38	1.34
22	BA	821	A	N3-C4	5.18	1.38	1.34
22	BA	460	A	N3-C4	5.17	1.38	1.34
22	BA	1304	A	N3-C4	5.17	1.38	1.34
22	BA	1700	A	N3-C4	5.17	1.38	1.34
22	BA	401	A	N7-C5	-5.17	1.36	1.39
22	BA	749	A	N3-C4	5.17	1.38	1.34
22	BA	14	A	N3-C4	5.17	1.38	1.34
22	BA	845	A	C2-N3	5.17	1.38	1.33
22	BA	896	A	C2-N3	5.17	1.38	1.33
22	BA	900	A	C2-N3	5.17	1.38	1.33
22	BA	1046	A	C2-N3	5.17	1.38	1.33
1	AA	51	A	N3-C4	5.17	1.38	1.34
1	AA	435	A	C2-N3	5.17	1.38	1.33
1	AA	383	A	N7-C5	-5.17	1.36	1.39
1	AA	1022	A	C2-N3	5.17	1.38	1.33
22	BA	1937	A	N3-C4	5.17	1.38	1.34
22	BA	2434	A	N3-C4	5.17	1.38	1.34
22	BA	2778	A	N7-C5	-5.17	1.36	1.39
22	BA	272	A	C2-N3	5.17	1.38	1.33
22	BA	2328	A	C8-N7	5.17	1.35	1.31
1	AA	1251	A	C2-N3	5.16	1.38	1.33
22	BA	1226	A	N3-C4	5.16	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1998	A	N7-C5	-5.16	1.36	1.39
22	BA	2183	A	C2-N3	5.16	1.38	1.33
1	AA	315	A	C2-N3	5.16	1.38	1.33
1	AA	456	A	C2-N3	5.16	1.38	1.33
22	BA	2134	A	C2-N3	5.16	1.38	1.33
22	BA	2336	A	N3-C4	5.16	1.38	1.34
22	BA	984	A	N7-C5	-5.16	1.36	1.39
55	B8	59	A	N3-C4	5.16	1.38	1.34
1	AA	478	A	C2-N3	5.16	1.38	1.33
22	BA	94	A	N3-C4	5.16	1.38	1.34
22	BA	1590	A	C2-N3	5.16	1.38	1.33
22	BA	1385	A	N3-C4	5.15	1.38	1.34
25	BD	152	PRO	CG-CD	-5.15	1.33	1.50
22	BA	196	A	N3-C4	5.15	1.38	1.34
22	BA	197	A	C8-N7	5.15	1.35	1.31
22	BA	727	A	C8-N7	5.15	1.35	1.31
22	BA	943	A	C8-N7	5.15	1.35	1.31
22	BA	2564	A	N3-C4	5.15	1.38	1.34
1	AA	1375	A	C2-N3	5.15	1.38	1.33
23	BB	94	A	N3-C4	5.15	1.38	1.34
22	BA	1085	A	C2-N3	5.15	1.38	1.33
1	AA	298	A	N3-C4	5.15	1.38	1.34
1	AA	432	A	C2-N3	5.15	1.38	1.33
22	BA	608	A	N3-C4	5.15	1.38	1.34
22	BA	2706	A	N7-C5	-5.15	1.36	1.39
1	AA	1150	A	C2-N3	5.14	1.38	1.33
22	BA	190	A	N3-C4	5.14	1.38	1.34
1	AA	1042	A	C2-N3	5.14	1.38	1.33
23	BB	119	A	C2-N3	5.14	1.38	1.33
22	BA	2284	A	N3-C4	5.14	1.38	1.34
1	AA	279	A	N3-C4	5.14	1.38	1.34
1	AA	1036	A	C2-N3	5.14	1.38	1.33
22	BA	503	A	N3-C4	5.14	1.38	1.34
1	AA	865	A	C2-N3	5.13	1.38	1.33
22	BA	480	A	N3-C4	5.13	1.38	1.34
22	BA	1048	A	C2-N3	5.13	1.38	1.33
22	BA	1580	A	C2-N3	5.13	1.38	1.33
1	AA	430	A	C2-N3	5.13	1.38	1.33
1	AA	1180	A	C2-N3	5.13	1.38	1.33
22	BA	74	A	N3-C4	5.13	1.38	1.34
22	BA	749	A	N7-C5	-5.13	1.36	1.39
22	BA	1803	A	C8-N7	5.13	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1374	A	C2-N3	5.13	1.38	1.33
1	AA	635	A	C2-N3	5.13	1.38	1.33
22	BA	761	A	C5-C4	-5.13	1.35	1.38
22	BA	1780	A	N3-C4	5.13	1.38	1.34
1	AA	181	A	C2-N3	5.13	1.38	1.33
1	AA	1044	A	C2-N3	5.13	1.38	1.33
22	BA	1528	A	N7-C5	-5.13	1.36	1.39
22	BA	2386	A	C8-N7	5.13	1.35	1.31
22	BA	1522	A	N3-C4	5.12	1.38	1.34
22	BA	1027	A	N3-C4	5.12	1.38	1.34
22	BA	1155	A	N7-C5	-5.12	1.36	1.39
22	BA	1571	A	N7-C5	-5.12	1.36	1.39
22	BA	508	A	C2-N3	5.12	1.38	1.33
22	BA	609	A	C8-N7	5.12	1.35	1.31
22	BA	960	A	C2-N3	5.12	1.38	1.33
22	BA	2675	A	N3-C4	5.12	1.38	1.34
22	BA	556	A	N3-C4	5.12	1.38	1.34
22	BA	1029	A	C2-N3	5.12	1.38	1.33
22	BA	1532	A	C2-N3	5.12	1.38	1.33
1	AA	996	A	C2-N3	5.12	1.38	1.33
1	AA	1005	A	C2-N3	5.12	1.38	1.33
1	AA	1398	A	N3-C4	5.12	1.38	1.34
22	BA	878	A	C2-N3	5.12	1.38	1.33
22	BA	892	A	C2-N3	5.12	1.38	1.33
22	BA	1254	A	N7-C5	-5.12	1.36	1.39
1	AA	815	A	N3-C4	5.12	1.38	1.34
22	BA	196	A	N7-C5	-5.12	1.36	1.39
1	AA	1333	A	C2-N3	5.11	1.38	1.33
1	AA	1349	A	C2-N3	5.11	1.38	1.33
1	AA	923	A	C2-N3	5.11	1.38	1.33
22	BA	279	A	C2-N3	5.11	1.38	1.33
22	BA	1365	A	N3-C4	5.11	1.38	1.34
22	BA	2147	A	C2-N3	5.11	1.38	1.33
1	AA	539	A	C2-N3	5.11	1.38	1.33
1	AA	72	A	C2-N3	5.11	1.38	1.33
1	AA	901	A	C2-N3	5.11	1.38	1.33
2	AB	205	ASP	CB-CG	5.11	1.62	1.51
22	BA	282	A	C2-N3	5.11	1.38	1.33
1	AA	681	A	C2-N3	5.10	1.38	1.33
1	AA	964	A	C2-N3	5.10	1.38	1.33
22	BA	2135	A	C2-N3	5.10	1.38	1.33
22	BA	2426	A	N3-C4	5.10	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2776	A	N7-C5	-5.10	1.36	1.39
22	BA	2497	A	C8-N7	5.10	1.35	1.31
1	AA	250	A	C2-N3	5.10	1.38	1.33
1	AA	1280	A	C2-N3	5.10	1.38	1.33
1	AA	80	A	C2-N3	5.10	1.38	1.33
1	AA	374	A	C2-N3	5.10	1.38	1.33
22	BA	1848	A	C2-N3	5.10	1.38	1.33
1	AA	608	A	C2-N3	5.09	1.38	1.33
22	BA	142	A	C2-N3	5.09	1.38	1.33
22	BA	348	A	C2-N3	5.09	1.38	1.33
22	BA	1084	A	C2-N3	5.09	1.38	1.33
22	BA	1690	A	N3-C4	5.09	1.38	1.34
1	AA	28	A	C2-N3	5.09	1.38	1.33
1	AA	831	A	C2-N3	5.09	1.38	1.33
1	AA	1306	A	C2-N3	5.09	1.38	1.33
22	BA	668	A	N3-C4	5.09	1.38	1.34
22	BA	1495	A	N3-C4	5.09	1.38	1.34
22	BA	1854	A	C8-N7	5.09	1.35	1.31
22	BA	1111	A	C2-N3	5.09	1.38	1.33
22	BA	1287	A	C8-N7	5.09	1.35	1.31
22	BA	1469	A	C2-N3	5.09	1.38	1.33
1	AA	1357	A	C2-N3	5.09	1.38	1.33
1	AA	572	A	N3-C4	5.08	1.38	1.34
22	BA	218	A	C2-N3	5.08	1.38	1.33
1	AA	288	A	C2-N3	5.08	1.38	1.33
1	AA	1252	A	C2-N3	5.08	1.38	1.33
22	BA	482	A	C2-N3	5.08	1.38	1.33
22	BA	532	A	N7-C5	-5.08	1.36	1.39
55	B8	26	A	N3-C4	5.08	1.37	1.34
22	BA	223	A	N3-C4	5.08	1.37	1.34
22	BA	2675	A	N7-C5	-5.08	1.36	1.39
1	AA	192	A	C2-N3	5.08	1.38	1.33
1	AA	205	A	C2-N3	5.08	1.38	1.33
22	BA	156	A	C2-N3	5.08	1.38	1.33
22	BA	368	A	C2-N3	5.08	1.38	1.33
22	BA	829	A	N3-C4	5.08	1.37	1.34
22	BA	2054	A	C8-N7	5.08	1.35	1.31
22	BA	2900	A	C2-N3	5.08	1.38	1.33
1	AA	845	A	C2-N3	5.08	1.38	1.33
1	AA	935	A	C2-N3	5.08	1.38	1.33
1	AA	1428	A	N3-C4	5.08	1.37	1.34
22	BA	449	A	N3-C4	5.08	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	947	A	N7-C5	-5.08	1.36	1.39
22	BA	2071	A	C8-N7	5.08	1.35	1.31
22	BA	2721	A	N7-C5	-5.08	1.36	1.39
1	AA	523	A	C2-N3	5.07	1.38	1.33
22	BA	126	A	N3-C4	5.07	1.37	1.34
22	BA	1307	A	N3-C4	5.07	1.37	1.34
1	AA	1418	A	N7-C5	-5.07	1.36	1.39
22	BA	529	A	N3-C4	5.07	1.37	1.34
22	BA	2792	A	C2-N3	5.07	1.38	1.33
22	BA	715	A	C2-N3	5.07	1.38	1.33
22	BA	1586	A	C2-N3	5.07	1.38	1.33
22	BA	743	A	N7-C5	-5.07	1.36	1.39
22	BA	911	A	N7-C5	-5.06	1.36	1.39
1	AA	279	A	C2-N3	5.06	1.38	1.33
22	BA	1213	A	N3-C4	5.06	1.37	1.34
1	AA	743	A	C2-N3	5.06	1.38	1.33
22	BA	1366	A	N7-C5	-5.06	1.36	1.39
1	AA	946	A	C2-N3	5.06	1.38	1.33
1	AA	1289	A	C2-N3	5.06	1.38	1.33
1	AA	649	A	C2-N3	5.05	1.38	1.33
22	BA	354	A	C2-N3	5.05	1.38	1.33
22	BA	1808	A	N3-C4	5.05	1.37	1.34
1	AA	629	A	C2-N3	5.05	1.38	1.33
1	AA	718	A	C2-N3	5.05	1.38	1.33
1	AA	983	A	C2-N3	5.05	1.38	1.33
1	AA	1021	A	C2-N3	5.05	1.38	1.33
22	BA	582	A	C8-N7	5.05	1.35	1.31
22	BA	675	A	N3-C4	5.05	1.37	1.34
22	BA	750	A	N7-C5	-5.05	1.36	1.39
1	AA	143	A	C2-N3	5.05	1.38	1.33
22	BA	2412	A	C2-N3	5.05	1.38	1.33
22	BA	255	A	C8-N7	5.04	1.35	1.31
22	BA	1749	A	N3-C4	5.04	1.37	1.34
22	BA	2589	A	N3-C4	5.04	1.37	1.34
22	BA	1847	A	C2-N3	5.04	1.38	1.33
22	BA	1871	A	C2-N3	5.04	1.38	1.33
23	BB	66	A	N3-C4	5.04	1.37	1.34
1	AA	411	A	C2-N3	5.04	1.38	1.33
1	AA	1269	A	C2-N3	5.04	1.38	1.33
22	BA	1069	A	C2-N3	5.04	1.38	1.33
22	BA	1927	A	N3-C4	5.04	1.37	1.34
22	BA	2114	A	C2-N3	5.04	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	216	A	N7-C5	-5.04	1.36	1.39
1	AA	1534	A	C2-N3	5.04	1.38	1.33
22	BA	454	A	N3-C4	5.04	1.37	1.34
22	BA	1265	A	N3-C4	5.04	1.37	1.34
22	BA	1854	A	C2-N3	5.04	1.38	1.33
22	BA	2602	A	C2-N3	5.04	1.38	1.33
22	BA	2879	A	N7-C5	-5.04	1.36	1.39
1	AA	1093	A	C2-N3	5.04	1.38	1.33
22	BA	470	A	N3-C4	5.04	1.37	1.34
23	BB	57	A	C2-N3	5.04	1.38	1.33
1	AA	1254	A	C2-N3	5.04	1.38	1.33
1	AA	1493	A	C2-N3	5.04	1.38	1.33
22	BA	453	A	N7-C5	-5.04	1.36	1.39
22	BA	1938	A	N3-C4	5.04	1.37	1.34
1	AA	59	A	C2-N3	5.03	1.38	1.33
22	BA	1759	A	N3-C4	5.03	1.37	1.34
1	AA	1155	A	C2-N3	5.03	1.38	1.33
22	BA	217	A	N7-C5	-5.03	1.36	1.39
22	BA	340	A	N3-C4	5.03	1.37	1.34
22	BA	959	A	C8-N7	5.03	1.35	1.31
22	BA	1040	A	C2-N3	5.03	1.38	1.33
22	BA	1050	A	C2-N3	5.03	1.38	1.33
22	BA	1916	A	C2-N3	5.03	1.38	1.33
22	BA	2171	A	C2-N3	5.03	1.38	1.33
1	AA	655	A	C2-N3	5.03	1.38	1.33
22	BA	415	A	N7-C5	-5.03	1.36	1.39
22	BA	699	A	N7-C5	-5.03	1.36	1.39
22	BA	44	A	C2-N3	5.02	1.38	1.33
23	BB	73	A	C2-N3	5.02	1.38	1.33
1	AA	1363	A	C2-N3	5.02	1.38	1.33
22	BA	2531	A	C2-N3	5.02	1.38	1.33
22	BA	1142	A	N3-C4	5.02	1.37	1.34
1	AA	465	A	C2-N3	5.02	1.38	1.33
22	BA	278	A	C2-N3	5.02	1.38	1.33
1	AA	139	A	C2-N3	5.02	1.38	1.33
1	AA	298	A	C2-N3	5.02	1.38	1.33
1	AA	1318	A	C2-N3	5.02	1.38	1.33
22	BA	21	A	C2-N3	5.02	1.38	1.33
1	AA	109	A	N3-C4	5.01	1.37	1.34
1	AA	452	A	C2-N3	5.01	1.38	1.33
1	AA	1324	A	C2-N3	5.01	1.38	1.33
7	AG	2	PRO	CG-CD	-5.01	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	81	A	C2-N3	5.01	1.38	1.33
22	BA	1413	A	C2-N3	5.01	1.38	1.33
22	BA	980	A	N3-C4	5.01	1.37	1.34
22	BA	1214	A	N3-C4	5.01	1.37	1.34
22	BA	1626	A	N3-C4	5.01	1.37	1.34
22	BA	2407	A	N3-C4	5.01	1.37	1.34
1	AA	1368	A	C2-N3	5.01	1.38	1.33
22	BA	1593	A	C2-N3	5.01	1.38	1.33
1	AA	509	A	C2-N3	5.01	1.38	1.33
22	BA	2309	A	C2-N3	5.01	1.38	1.33
22	BA	586	A	N3-C4	5.01	1.37	1.34
22	BA	1641	A	C2-N3	5.01	1.38	1.33
22	BA	1928	A	N3-C4	5.01	1.37	1.34
1	AA	596	A	C2-N3	5.00	1.38	1.33
1	AA	860	A	C2-N3	5.00	1.38	1.33
22	BA	1953	A	N3-C4	5.00	1.37	1.34
1	AA	1531	A	C2-N3	5.00	1.38	1.33
22	BA	632	A	N3-C4	5.00	1.37	1.34
22	BA	1067	A	C2-N3	5.00	1.38	1.33
22	BA	2054	A	N7-C5	-5.00	1.36	1.39

All (12263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2872	A	N1-C6-N6	-26.13	102.92	118.60
22	BA	1848	A	N1-C6-N6	-22.75	104.95	118.60
22	BA	1285	A	N1-C6-N6	-22.74	104.95	118.60
22	BA	1253	A	N1-C6-N6	-22.72	104.97	118.60
1	AA	1299	A	N1-C6-N6	-22.71	104.97	118.60
1	AA	1446	A	N1-C6-N6	-22.59	105.05	118.60
22	BA	515	A	N1-C6-N6	-22.48	105.11	118.60
22	BA	1434	A	N1-C6-N6	-22.29	105.22	118.60
1	AA	1332	A	N1-C6-N6	-22.28	105.23	118.60
22	BA	1000	A	N1-C6-N6	-22.23	105.26	118.60
22	BA	941	A	N1-C6-N6	-22.19	105.28	118.60
22	BA	699	A	N1-C6-N6	-22.00	105.40	118.60
22	BA	13	A	N1-C6-N6	-21.99	105.40	118.60
22	BA	764	A	N1-C6-N6	-21.98	105.41	118.60
22	BA	2726	A	N1-C6-N6	-21.90	105.46	118.60
22	BA	782	A	N1-C6-N6	-21.87	105.48	118.60
22	BA	119	A	N1-C6-N6	-21.86	105.48	118.60
22	BA	479	A	N1-C6-N6	-21.85	105.49	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1214	A	N1-C6-N6	-21.80	105.52	118.60
22	BA	207	A	N1-C6-N6	-21.78	105.53	118.60
22	BA	783	A	N1-C6-N6	-21.73	105.56	118.60
22	BA	563	A	N1-C6-N6	-21.64	105.61	118.60
1	AA	1446	A	C2-N3-C4	21.59	121.39	110.60
22	BA	2882	A	N1-C6-N6	-21.58	105.66	118.60
22	BA	1853	A	N1-C6-N6	-21.57	105.66	118.60
22	BA	804	A	N1-C6-N6	-21.57	105.66	118.60
22	BA	1000	A	C2-N3-C4	21.56	121.38	110.60
22	BA	781	A	N1-C6-N6	-21.55	105.67	118.60
22	BA	529	A	N1-C6-N6	-21.53	105.68	118.60
22	BA	2598	A	N1-C6-N6	-21.53	105.68	118.60
22	BA	586	A	N1-C6-N6	-21.49	105.70	118.60
22	BA	2060	A	N1-C2-N3	-21.48	118.56	129.30
2	AB	188	ASP	CB-CG-OD1	21.47	137.62	118.30
22	BA	502	A	N1-C6-N6	-21.43	105.74	118.60
1	AA	412	A	N1-C6-N6	-21.40	105.76	118.60
22	BA	621	A	N1-C6-N6	-21.39	105.77	118.60
22	BA	1787	A	C2-N3-C4	21.37	121.28	110.60
1	AA	465	A	N1-C6-N6	-21.37	105.78	118.60
22	BA	165	A	N1-C6-N6	-21.35	105.79	118.60
22	BA	1668	A	N1-C6-N6	-21.31	105.81	118.60
1	AA	431	A	N1-C6-N6	-21.29	105.83	118.60
22	BA	782	A	C2-N3-C4	21.26	121.23	110.60
1	AA	1213	A	N1-C6-N6	-21.25	105.85	118.60
22	BA	457	A	N1-C6-N6	-21.20	105.88	118.60
1	AA	1004	A	N1-C6-N6	-21.19	105.89	118.60
22	BA	752	A	N1-C6-N6	-21.18	105.89	118.60
22	BA	2060	A	N1-C6-N6	-21.14	105.92	118.60
22	BA	1937	A	N1-C6-N6	-21.13	105.92	118.60
22	BA	2566	A	N1-C2-N3	-21.12	118.74	129.30
22	BA	2590	A	N1-C6-N6	-21.11	105.93	118.60
22	BA	2005	A	N1-C6-N6	-21.11	105.94	118.60
22	BA	2764	A	N1-C6-N6	-21.10	105.94	118.60
22	BA	1819	A	N1-C6-N6	-21.09	105.94	118.60
22	BA	2810	A	N1-C6-N6	-21.08	105.95	118.60
22	BA	2826	A	N1-C6-N6	-21.03	105.98	118.60
22	BA	1286	A	N1-C6-N6	-21.01	106.00	118.60
22	BA	794	A	C2-N3-C4	20.99	121.09	110.60
22	BA	1353	A	N1-C6-N6	-20.98	106.01	118.60
1	AA	1447	A	N1-C6-N6	-20.98	106.01	118.60
1	AA	889	A	N1-C6-N6	-20.96	106.03	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1544	A	N1-C6-N6	-20.94	106.04	118.60
22	BA	310	A	N1-C6-N6	-20.93	106.04	118.60
1	AA	704	A	N1-C6-N6	-20.93	106.04	118.60
1	AA	313	A	C2-N3-C4	20.89	121.05	110.60
22	BA	2541	A	N1-C6-N6	-20.88	106.07	118.60
1	AA	665	A	N1-C6-N6	-20.87	106.08	118.60
22	BA	466	A	N1-C6-N6	-20.87	106.08	118.60
22	BA	1632	A	N1-C6-N6	-20.83	106.10	118.60
22	BA	2406	A	N1-C6-N6	-20.83	106.10	118.60
22	BA	675	A	N1-C6-N6	-20.83	106.10	118.60
22	BA	2430	A	N1-C6-N6	-20.83	106.11	118.60
22	BA	84	A	N1-C6-N6	-20.82	106.11	118.60
22	BA	322	A	N1-C6-N6	-20.81	106.11	118.60
22	BA	478	A	N1-C6-N6	-20.81	106.11	118.60
22	BA	241	A	N1-C6-N6	-20.81	106.12	118.60
22	BA	1569	A	N1-C6-N6	-20.80	106.12	118.60
22	BA	2448	A	N1-C6-N6	-20.79	106.13	118.60
1	AA	1239	A	N1-C6-N6	-20.78	106.13	118.60
22	BA	2758	A	N1-C6-N6	-20.76	106.15	118.60
1	AA	461	A	C2-N3-C4	20.73	120.97	110.60
22	BA	979	A	N1-C6-N6	-20.71	106.17	118.60
22	BA	984	A	N1-C6-N6	-20.71	106.17	118.60
1	AA	1340	A	N1-C2-N3	-20.71	118.95	129.30
22	BA	2835	A	N1-C6-N6	-20.70	106.18	118.60
22	BA	1650	A	C2-N3-C4	20.69	120.95	110.60
22	BA	514	A	N1-C6-N6	-20.66	106.20	118.60
1	AA	1500	A	C2-N3-C4	20.66	120.93	110.60
22	BA	973	A	N1-C6-N6	-20.64	106.21	118.60
22	BA	1630	A	N1-C6-N6	-20.61	106.23	118.60
22	BA	1789	A	N1-C6-N6	-20.61	106.23	118.60
22	BA	207	A	C2-N3-C4	20.60	120.90	110.60
1	AA	777	A	N1-C6-N6	-20.59	106.25	118.60
22	BA	2614	A	C2-N3-C4	20.59	120.89	110.60
22	BA	1545	A	N1-C6-N6	-20.57	106.26	118.60
22	BA	2450	A	N1-C6-N6	-20.56	106.26	118.60
22	BA	1655	A	N1-C6-N6	-20.56	106.27	118.60
1	AA	152	A	N1-C6-N6	-20.54	106.28	118.60
22	BA	1392	A	N1-C6-N6	-20.54	106.28	118.60
22	BA	761	A	N1-C6-N6	-20.54	106.28	118.60
22	BA	689	A	C2-N3-C4	20.53	120.86	110.60
22	BA	1821	A	N1-C6-N6	-20.52	106.29	118.60
22	BA	2273	A	C2-N3-C4	20.51	120.86	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2060	A	C2-N3-C4	20.51	120.86	110.60
22	BA	160	A	N1-C6-N6	-20.51	106.30	118.60
22	BA	1395	A	N1-C6-N6	-20.50	106.30	118.60
22	BA	563	A	C2-N3-C4	20.50	120.85	110.60
22	BA	2749	A	N1-C6-N6	-20.49	106.30	118.60
22	BA	2542	A	N1-C6-N6	-20.49	106.31	118.60
1	AA	915	A	N1-C6-N6	-20.47	106.32	118.60
22	BA	2572	A	N1-C6-N6	-20.47	106.32	118.60
22	BA	504	A	N1-C2-N3	-20.44	119.08	129.30
22	BA	783	A	C2-N3-C4	20.44	120.82	110.60
22	BA	1754	A	N1-C6-N6	-20.43	106.34	118.60
22	BA	1204	A	N1-C6-N6	-20.43	106.34	118.60
22	BA	1598	A	N1-C6-N6	-20.42	106.35	118.60
22	BA	1028	A	N1-C2-N3	-20.42	119.09	129.30
22	BA	84	A	N1-C2-N3	-20.41	119.09	129.30
22	BA	677	A	C2-N3-C4	20.41	120.81	110.60
22	BA	1889	A	N1-C6-N6	-20.41	106.36	118.60
1	AA	1500	A	N1-C6-N6	-20.41	106.36	118.60
22	BA	479	A	N1-C2-N3	-20.40	119.10	129.30
22	BA	1655	A	N1-C2-N3	-20.39	119.11	129.30
22	BA	217	A	N1-C6-N6	-20.37	106.38	118.60
22	BA	2033	A	N1-C6-N6	-20.37	106.38	118.60
22	BA	1392	A	C2-N3-C4	20.36	120.78	110.60
1	AA	151	A	N1-C6-N6	-20.36	106.38	118.60
22	BA	1308	A	N1-C6-N6	-20.36	106.38	118.60
22	BA	1156	A	N1-C6-N6	-20.35	106.39	118.60
22	BA	1515	A	N1-C6-N6	-20.34	106.39	118.60
22	BA	685	A	C2-N3-C4	20.33	120.77	110.60
22	BA	1754	A	N1-C2-N3	-20.33	119.14	129.30
22	BA	2281	A	C2-N3-C4	20.32	120.76	110.60
22	BA	10	A	N1-C6-N6	-20.30	106.42	118.60
22	BA	750	A	C2-N3-C4	20.29	120.75	110.60
22	BA	734	A	N1-C6-N6	-20.29	106.43	118.60
1	AA	958	A	N1-C6-N6	-20.28	106.43	118.60
1	AA	1340	A	N1-C6-N6	-20.28	106.44	118.60
1	AA	460	A	C2-N3-C4	20.27	120.74	110.60
22	BA	1544	A	C2-N3-C4	20.26	120.73	110.60
1	AA	819	A	N1-C6-N6	-20.25	106.45	118.60
22	BA	1598	A	C2-N3-C4	20.24	120.72	110.60
1	AA	459	A	C2-N3-C4	20.23	120.72	110.60
22	BA	111	A	N1-C6-N6	-20.23	106.47	118.60
22	BA	2781	A	N1-C2-N3	-20.21	119.19	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1655	A	C2-N3-C4	20.20	120.70	110.60
22	BA	1205	A	N1-C6-N6	-20.20	106.48	118.60
22	BA	1998	A	C2-N3-C4	20.20	120.70	110.60
22	BA	1603	A	C2-N3-C4	20.19	120.69	110.60
22	BA	1848	A	C2-N3-C4	20.18	120.69	110.60
22	BA	1789	A	N1-C2-N3	-20.17	119.22	129.30
22	BA	2451	A	C2-N3-C4	20.17	120.68	110.60
22	BA	279	A	N1-C6-N6	-20.16	106.51	118.60
22	BA	1253	A	C2-N3-C4	20.15	120.67	110.60
22	BA	1819	A	C2-N3-C4	20.15	120.67	110.60
22	BA	2565	A	N1-C6-N6	-20.15	106.51	118.60
22	BA	1890	A	N1-C6-N6	-20.15	106.51	118.60
23	BB	46	A	N1-C6-N6	-20.15	106.51	118.60
22	BA	2776	A	N1-C6-N6	-20.14	106.51	118.60
22	BA	2080	A	C2-N3-C4	20.14	120.67	110.60
22	BA	332	A	N1-C6-N6	-20.14	106.52	118.60
22	BA	126	A	N1-C2-N3	-20.13	119.24	129.30
22	BA	1439	A	N1-C6-N6	-20.12	106.53	118.60
22	BA	2469	A	C2-N3-C4	20.12	120.66	110.60
1	AA	120	A	N1-C6-N6	-20.11	106.53	118.60
22	BA	203	A	N1-C6-N6	-20.11	106.53	118.60
1	AA	1238	A	N1-C6-N6	-20.10	106.54	118.60
22	BA	457	A	N1-C2-N3	-20.10	119.25	129.30
22	BA	1551	A	N1-C6-N6	-20.10	106.54	118.60
22	BA	1214	A	C2-N3-C4	20.09	120.64	110.60
22	BA	1853	A	N1-C2-N3	-20.08	119.26	129.30
1	AA	802	A	N1-C6-N6	-20.07	106.56	118.60
22	BA	782	A	N1-C2-N3	-20.07	119.27	129.30
22	BA	1378	A	N1-C6-N6	-20.06	106.56	118.60
1	AA	59	A	N1-C6-N6	-20.05	106.57	118.60
22	BA	195	A	C2-N3-C4	20.04	120.62	110.60
22	BA	1156	A	N1-C2-N3	-20.03	119.28	129.30
22	BA	802	A	C2-N3-C4	20.02	120.61	110.60
22	BA	2199	A	N1-C6-N6	-20.02	106.59	118.60
22	BA	514	A	N1-C2-N3	-20.01	119.29	129.30
22	BA	1570	A	N1-C6-N6	-20.00	106.60	118.60
1	AA	1004	A	C2-N3-C4	20.00	120.60	110.60
22	BA	1275	A	N1-C6-N6	-19.99	106.60	118.60
22	BA	2753	A	N1-C6-N6	-19.99	106.61	118.60
22	BA	1597	A	N1-C6-N6	-19.98	106.61	118.60
22	BA	1366	A	N1-C6-N6	-19.98	106.61	118.60
1	AA	26	A	N1-C6-N6	-19.98	106.61	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	216	A	N1-C6-N6	-19.98	106.61	118.60
1	AA	274	A	N1-C2-N3	-19.97	119.32	129.30
22	BA	2837	A	N1-C6-N6	-19.96	106.62	118.60
1	AA	363	A	N1-C6-N6	-19.96	106.62	118.60
22	BA	927	A	N1-C6-N6	-19.96	106.62	118.60
22	BA	1253	A	N1-C2-N3	-19.96	119.32	129.30
22	BA	529	A	N1-C2-N3	-19.96	119.32	129.30
22	BA	1808	A	N1-C6-N6	-19.96	106.62	118.60
22	BA	621	A	C2-N3-C4	19.96	120.58	110.60
22	BA	2273	A	N1-C2-N3	-19.94	119.33	129.30
22	BA	478	A	C2-N3-C4	19.94	120.57	110.60
22	BA	2837	A	C2-N3-C4	19.94	120.57	110.60
22	BA	1791	A	N1-C6-N6	-19.93	106.64	118.60
22	BA	988	A	N1-C6-N6	-19.92	106.65	118.60
22	BA	270	A	N1-C6-N6	-19.91	106.65	118.60
22	BA	2741	A	N1-C6-N6	-19.91	106.66	118.60
1	AA	1502	A	N1-C6-N6	-19.90	106.66	118.60
22	BA	1165	A	N1-C2-N3	-19.89	119.36	129.30
22	BA	608	A	N1-C2-N3	-19.89	119.36	129.30
22	BA	800	A	N1-C6-N6	-19.89	106.67	118.60
1	AA	16	A	N1-C6-N6	-19.88	106.67	118.60
22	BA	1353	A	C2-N3-C4	19.86	120.53	110.60
1	AA	906	A	N1-C6-N6	-19.86	106.68	118.60
22	BA	608	A	C2-N3-C4	19.85	120.53	110.60
22	BA	309	A	N1-C6-N6	-19.85	106.69	118.60
22	BA	637	A	N1-C2-N3	-19.85	119.38	129.30
22	BA	191	A	C2-N3-C4	19.85	120.52	110.60
1	AA	676	A	N1-C6-N6	-19.84	106.69	118.60
22	BA	1640	A	C2-N3-C4	19.84	120.52	110.60
22	BA	2740	A	C2-N3-C4	19.84	120.52	110.60
1	AA	253	A	N1-C6-N6	-19.84	106.69	118.60
22	BA	1791	A	C2-N3-C4	19.84	120.52	110.60
1	AA	792	A	N1-C6-N6	-19.83	106.70	118.60
1	AA	825	A	N1-C6-N6	-19.82	106.70	118.60
22	BA	497	A	N1-C6-N6	-19.82	106.71	118.60
22	BA	2873	A	N1-C6-N6	-19.82	106.71	118.60
22	BA	2005	A	C2-N3-C4	19.81	120.50	110.60
22	BA	905	A	N1-C6-N6	-19.80	106.72	118.60
22	BA	1853	A	C2-N3-C4	19.80	120.50	110.60
22	BA	572	A	C2-N3-C4	19.80	120.50	110.60
22	BA	1772	A	C2-N3-C4	19.80	120.50	110.60
22	BA	71	A	N1-C6-N6	-19.80	106.72	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1322	A	N1-C2-N3	-19.80	119.40	129.30
22	BA	244	A	C2-N3-C4	19.80	120.50	110.60
22	BA	2883	A	N1-C6-N6	-19.80	106.72	118.60
1	AA	996	A	N1-C6-N6	-19.79	106.72	118.60
22	BA	222	A	N1-C6-N6	-19.79	106.72	118.60
22	BA	2451	A	N1-C6-N6	-19.79	106.72	118.60
23	BB	59	A	C2-N3-C4	19.79	120.50	110.60
1	AA	498	A	C2-N3-C4	19.78	120.49	110.60
22	BA	2014	A	N1-C6-N6	-19.78	106.73	118.60
1	AA	1346	A	N1-C6-N6	-19.78	106.73	118.60
22	BA	1028	A	C2-N3-C4	19.78	120.49	110.60
55	B8	41	A	N1-C6-N6	-19.78	106.73	118.60
1	AA	195	A	N1-C6-N6	-19.77	106.74	118.60
22	BA	532	A	N1-C6-N6	-19.77	106.74	118.60
22	BA	199	A	N1-C6-N6	-19.77	106.74	118.60
22	BA	262	A	N1-C6-N6	-19.77	106.74	118.60
22	BA	1672	A	N1-C6-N6	-19.77	106.74	118.60
22	BA	221	A	N1-C2-N3	-19.76	119.42	129.30
22	BA	160	A	C2-N3-C4	19.76	120.48	110.60
1	AA	938	A	C2-N3-C4	19.76	120.48	110.60
22	BA	1439	A	C2-N3-C4	19.76	120.48	110.60
22	BA	1586	A	N1-C6-N6	-19.76	106.75	118.60
22	BA	1936	A	C2-N3-C4	19.76	120.48	110.60
22	BA	1847	A	C2-N3-C4	19.75	120.48	110.60
22	BA	21	A	C2-N3-C4	19.75	120.48	110.60
22	BA	685	A	N1-C6-N6	-19.75	106.75	118.60
22	BA	1783	A	N1-C2-N3	-19.75	119.42	129.30
1	AA	44	A	N1-C6-N6	-19.75	106.75	118.60
22	BA	1001	A	N1-C6-N6	-19.74	106.76	118.60
22	BA	2589	A	N1-C6-N6	-19.73	106.76	118.60
1	AA	919	A	N1-C6-N6	-19.73	106.76	118.60
1	AA	918	A	N1-C6-N6	-19.73	106.76	118.60
22	BA	1762	A	N1-C6-N6	-19.73	106.77	118.60
22	BA	1970	A	N1-C2-N3	-19.73	119.44	129.30
22	BA	1936	A	N1-C2-N3	-19.72	119.44	129.30
1	AA	1476	A	N1-C6-N6	-19.72	106.77	118.60
1	AA	151	A	C2-N3-C4	19.72	120.46	110.60
22	BA	191	A	N1-C6-N6	-19.71	106.77	118.60
55	B8	58	A	N1-C2-N3	-19.71	119.44	129.30
22	BA	1244	A	C2-N3-C4	19.71	120.45	110.60
23	BB	78	A	N1-C6-N6	-19.70	106.78	118.60
22	BA	621	A	N1-C2-N3	-19.69	119.45	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	460	A	N1-C6-N6	-19.69	106.78	118.60
23	BB	101	A	N1-C6-N6	-19.68	106.79	118.60
22	BA	1189	A	C2-N3-C4	19.68	120.44	110.60
22	BA	825	A	C2-N3-C4	19.68	120.44	110.60
22	BA	959	A	N1-C2-N3	-19.68	119.46	129.30
22	BA	2358	A	N1-C6-N6	-19.68	106.79	118.60
22	BA	342	A	N1-C6-N6	-19.67	106.80	118.60
22	BA	825	A	N1-C6-N6	-19.67	106.80	118.60
55	B8	42	A	C2-N3-C4	19.67	120.44	110.60
22	BA	602	A	N1-C6-N6	-19.67	106.80	118.60
22	BA	2003	A	C2-N3-C4	19.67	120.43	110.60
22	BA	972	A	C2-N3-C4	19.66	120.43	110.60
22	BA	1420	A	N1-C6-N6	-19.66	106.81	118.60
1	AA	935	A	N1-C6-N6	-19.65	106.81	118.60
1	AA	282	A	N1-C6-N6	-19.64	106.81	118.60
22	BA	2682	A	N1-C6-N6	-19.64	106.82	118.60
1	AA	520	A	N1-C6-N6	-19.64	106.82	118.60
22	BA	507	A	N1-C2-N3	-19.64	119.48	129.30
22	BA	449	A	C2-N3-C4	19.63	120.42	110.60
22	BA	2700	A	C2-N3-C4	19.63	120.42	110.60
22	BA	1755	A	C2-N3-C4	19.63	120.41	110.60
22	BA	2266	A	C2-N3-C4	19.63	120.41	110.60
1	AA	900	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	1265	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	2469	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	1129	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	973	A	C2-N3-C4	19.62	120.41	110.60
22	BA	1672	A	C2-N3-C4	19.62	120.41	110.60
1	AA	872	A	C2-N3-C4	19.61	120.41	110.60
22	BA	1392	A	N1-C2-N3	-19.61	119.49	129.30
22	BA	981	A	N1-C2-N3	-19.61	119.49	129.30
22	BA	1755	A	N1-C6-N6	-19.61	106.83	118.60
1	AA	553	A	C2-N3-C4	19.61	120.40	110.60
22	BA	262	A	C2-N3-C4	19.61	120.40	110.60
22	BA	1268	A	C2-N3-C4	19.61	120.40	110.60
22	BA	1755	A	N1-C2-N3	-19.61	119.50	129.30
1	AA	909	A	N1-C6-N6	-19.61	106.84	118.60
22	BA	2198	A	N1-C2-N3	-19.61	119.50	129.30
1	AA	482	A	N1-C6-N6	-19.60	106.84	118.60
1	AA	753	A	N1-C6-N6	-19.60	106.84	118.60
22	BA	2327	A	C2-N3-C4	19.60	120.40	110.60
23	BB	101	A	C2-N3-C4	19.60	120.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	766	A	N1-C6-N6	-19.59	106.84	118.60
1	AA	1299	A	C2-N3-C4	19.59	120.40	110.60
22	BA	83	A	N1-C6-N6	-19.59	106.84	118.60
22	BA	2721	A	N1-C6-N6	-19.59	106.85	118.60
22	BA	2198	A	N1-C6-N6	-19.59	106.85	118.60
1	AA	1287	A	N1-C6-N6	-19.58	106.85	118.60
22	BA	1679	A	C2-N3-C4	19.58	120.39	110.60
22	BA	990	A	N1-C6-N6	-19.57	106.86	118.60
1	AA	572	A	N1-C6-N6	-19.57	106.86	118.60
1	AA	253	A	C2-N3-C4	19.57	120.38	110.60
23	BB	53	A	N1-C6-N6	-19.57	106.86	118.60
22	BA	821	A	N1-C6-N6	-19.56	106.86	118.60
22	BA	2823	A	N1-C6-N6	-19.56	106.87	118.60
22	BA	2547	A	N1-C6-N6	-19.55	106.87	118.60
22	BA	1847	A	N1-C6-N6	-19.55	106.87	118.60
22	BA	2727	A	C2-N3-C4	19.55	120.38	110.60
1	AA	321	A	N1-C6-N6	-19.55	106.87	118.60
22	BA	727	A	N1-C2-N3	-19.55	119.53	129.30
22	BA	1287	A	C2-N3-C4	19.55	120.38	110.60
22	BA	213	A	C2-N3-C4	19.55	120.37	110.60
22	BA	1927	A	N1-C6-N6	-19.55	106.87	118.60
22	BA	2388	A	N1-C2-N3	-19.55	119.53	129.30
22	BA	1784	A	N1-C6-N6	-19.54	106.87	118.60
22	BA	2212	A	N1-C6-N6	-19.54	106.88	118.60
22	BA	423	A	C2-N3-C4	19.54	120.37	110.60
22	BA	222	A	N1-C2-N3	-19.54	119.53	129.30
1	AA	673	A	C2-N3-C4	19.53	120.37	110.60
22	BA	2634	A	C2-N3-C4	19.53	120.37	110.60
22	BA	2826	A	C2-N3-C4	19.53	120.37	110.60
22	BA	603	A	N1-C2-N3	-19.53	119.54	129.30
23	BB	109	A	N1-C6-N6	-19.52	106.89	118.60
1	AA	116	A	C2-N3-C4	19.52	120.36	110.60
1	AA	607	A	N1-C6-N6	-19.52	106.89	118.60
1	AA	274	A	C2-N3-C4	19.52	120.36	110.60
22	BA	443	A	N1-C6-N6	-19.52	106.89	118.60
22	BA	1032	A	N1-C6-N6	-19.52	106.89	118.60
22	BA	1427	A	N1-C6-N6	-19.52	106.89	118.60
22	BA	1608	A	C2-N3-C4	19.52	120.36	110.60
22	BA	1000	A	N1-C2-N3	-19.51	119.54	129.30
22	BA	2266	A	N1-C2-N3	-19.51	119.54	129.30
22	BA	213	A	N1-C2-N3	-19.51	119.55	129.30
22	BA	1194	A	N1-C6-N6	-19.51	106.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1608	A	N1-C6-N6	-19.50	106.90	118.60
22	BA	1287	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	1427	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	310	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	910	A	N1-C2-N3	-19.49	119.55	129.30
22	BA	1336	A	C2-N3-C4	19.49	120.35	110.60
22	BA	975	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	1786	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	2439	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	2281	A	N1-C6-N6	-19.48	106.92	118.60
22	BA	207	A	N1-C2-N3	-19.47	119.56	129.30
22	BA	602	A	N1-C2-N3	-19.47	119.56	129.30
22	BA	2542	A	C2-N3-C4	19.47	120.33	110.60
22	BA	195	A	N1-C6-N6	-19.46	106.92	118.60
22	BA	821	A	N1-C2-N3	-19.46	119.57	129.30
22	BA	532	A	C2-N3-C4	19.46	120.33	110.60
22	BA	1260	A	C2-N3-C4	19.45	120.33	110.60
22	BA	1165	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	918	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	2829	A	N1-C6-N6	-19.44	106.93	118.60
22	BA	2199	A	C2-N3-C4	19.44	120.32	110.60
1	AA	1311	A	N1-C6-N6	-19.44	106.94	118.60
1	AA	596	A	N1-C6-N6	-19.44	106.94	118.60
1	AA	1513	A	C2-N3-C4	19.44	120.32	110.60
22	BA	2052	A	N1-C6-N6	-19.44	106.94	118.60
1	AA	129	A	N1-C6-N6	-19.43	106.94	118.60
22	BA	599	A	C2-N3-C4	19.43	120.32	110.60
1	AA	792	A	N1-C2-N3	-19.43	119.58	129.30
1	AA	253	A	N1-C2-N3	-19.43	119.59	129.30
22	BA	2781	A	N1-C6-N6	-19.43	106.94	118.60
22	BA	2453	A	C2-N3-C4	19.42	120.31	110.60
22	BA	1246	A	N1-C6-N6	-19.42	106.95	118.60
22	BA	1165	A	C2-N3-C4	19.42	120.31	110.60
1	AA	408	A	N1-C6-N6	-19.42	106.95	118.60
22	BA	118	A	N1-C2-N3	-19.41	119.59	129.30
22	BA	739	A	N1-C2-N3	-19.41	119.59	129.30
1	AA	412	A	N1-C2-N3	-19.41	119.59	129.30
1	AA	621	A	C2-N3-C4	19.41	120.30	110.60
55	B8	66	A	N1-C2-N3	-19.41	119.60	129.30
22	BA	342	A	C2-N3-C4	19.41	120.30	110.60
22	BA	2738	A	N1-C2-N3	-19.41	119.60	129.30
1	AA	1500	A	N1-C2-N3	-19.40	119.60	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1268	A	N1-C2-N3	-19.40	119.60	129.30
22	BA	2031	A	N1-C2-N3	-19.40	119.60	129.30
22	BA	980	A	C2-N3-C4	19.39	120.30	110.60
22	BA	1525	A	N1-C6-N6	-19.39	106.96	118.60
22	BA	2031	A	C2-N3-C4	19.39	120.30	110.60
1	AA	1163	A	C2-N3-C4	19.39	120.29	110.60
22	BA	820	A	C2-N3-C4	19.39	120.29	110.60
22	BA	2614	A	N1-C6-N6	-19.39	106.97	118.60
22	BA	2726	A	C2-N3-C4	19.39	120.29	110.60
1	AA	1398	A	N1-C6-N6	-19.39	106.97	118.60
22	BA	2829	A	N1-C2-N3	-19.37	119.61	129.30
22	BA	2411	A	N1-C6-N6	-19.37	106.98	118.60
22	BA	764	A	N1-C2-N3	-19.37	119.61	129.30
23	BB	115	A	C2-N3-C4	19.37	120.29	110.60
22	BA	1086	A	N1-C6-N6	-19.37	106.98	118.60
1	AA	309	A	N1-C2-N3	-19.37	119.62	129.30
22	BA	675	A	C2-N3-C4	19.37	120.28	110.60
22	BA	2781	A	C2-N3-C4	19.37	120.28	110.60
22	BA	522	A	C2-N3-C4	19.37	120.28	110.60
22	BA	2748	A	N1-C6-N6	-19.36	106.98	118.60
22	BA	423	A	N1-C6-N6	-19.35	106.99	118.60
22	BA	1759	A	C2-N3-C4	19.35	120.28	110.60
22	BA	2572	A	N1-C2-N3	-19.35	119.63	129.30
1	AA	1092	A	N1-C6-N6	-19.35	106.99	118.60
1	AA	1180	A	N1-C6-N6	-19.34	106.99	118.60
22	BA	637	A	N1-C6-N6	-19.34	107.00	118.60
22	BA	631	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	983	A	N1-C2-N3	-19.33	119.63	129.30
1	AA	509	A	C2-N3-C4	19.33	120.27	110.60
22	BA	1496	A	N1-C2-N3	-19.33	119.64	129.30
22	BA	2513	A	C2-N3-C4	19.33	120.27	110.60
22	BA	1998	A	N1-C6-N6	-19.33	107.00	118.60
22	BA	2736	A	N1-C6-N6	-19.33	107.00	118.60
22	BA	685	A	N1-C2-N3	-19.32	119.64	129.30
22	BA	1570	A	C2-N3-C4	19.32	120.26	110.60
22	BA	278	A	C2-N3-C4	19.32	120.26	110.60
22	BA	330	A	C2-N3-C4	19.31	120.26	110.60
1	AA	172	A	N1-C6-N6	-19.31	107.01	118.60
22	BA	1214	A	N1-C2-N3	-19.31	119.64	129.30
22	BA	1632	A	C2-N3-C4	19.31	120.25	110.60
22	BA	149	A	N1-C6-N6	-19.31	107.02	118.60
22	BA	592	A	C2-N3-C4	19.31	120.25	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1912	A	N1-C6-N6	-19.31	107.02	118.60
22	BA	750	A	N1-C2-N3	-19.30	119.65	129.30
22	BA	2657	A	N1-C6-N6	-19.30	107.02	118.60
1	AA	1333	A	N1-C6-N6	-19.30	107.02	118.60
1	AA	320	A	N1-C6-N6	-19.30	107.02	118.60
1	AA	1428	A	N1-C6-N6	-19.30	107.02	118.60
1	AA	781	A	N1-C6-N6	-19.29	107.02	118.60
1	AA	397	A	C2-N3-C4	19.29	120.25	110.60
22	BA	2679	A	C2-N3-C4	19.29	120.25	110.60
22	BA	2879	A	N1-C6-N6	-19.29	107.03	118.60
22	BA	2212	A	C2-N3-C4	19.29	120.24	110.60
1	AA	72	A	N1-C6-N6	-19.28	107.03	118.60
1	AA	336	A	C2-N3-C4	19.28	120.24	110.60
22	BA	1603	A	N1-C2-N3	-19.28	119.66	129.30
22	BA	866	A	N1-C6-N6	-19.28	107.03	118.60
22	BA	959	A	C2-N3-C4	19.27	120.24	110.60
22	BA	2241	A	C2-N3-C4	19.27	120.24	110.60
22	BA	42	A	C2-N3-C4	19.27	120.23	110.60
22	BA	788	A	N1-C6-N6	-19.27	107.04	118.60
22	BA	1858	A	N1-C6-N6	-19.27	107.04	118.60
22	BA	661	A	C2-N3-C4	19.27	120.23	110.60
22	BA	753	A	C2-N3-C4	19.27	120.23	110.60
22	BA	1987	A	C2-N3-C4	19.27	120.23	110.60
22	BA	2868	A	C2-N3-C4	19.27	120.23	110.60
1	AA	466	A	N1-C6-N6	-19.26	107.04	118.60
22	BA	2542	A	N1-C2-N3	-19.26	119.67	129.30
22	BA	529	A	C2-N3-C4	19.26	120.23	110.60
22	BA	2340	A	C2-N3-C4	19.26	120.23	110.60
22	BA	1987	A	N1-C2-N3	-19.26	119.67	129.30
22	BA	716	A	N1-C2-N3	-19.25	119.67	129.30
22	BA	1522	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	1367	A	C2-N3-C4	19.25	120.23	110.60
1	AA	151	A	N1-C2-N3	-19.25	119.67	129.30
22	BA	221	A	C2-N3-C4	19.25	120.22	110.60
22	BA	119	A	N1-C2-N3	-19.25	119.68	129.30
22	BA	71	A	C2-N3-C4	19.24	120.22	110.60
22	BA	2406	A	N1-C2-N3	-19.24	119.68	129.30
1	AA	171	A	N1-C6-N6	-19.23	107.06	118.60
22	BA	1367	A	N1-C6-N6	-19.23	107.06	118.60
22	BA	1515	A	C2-N3-C4	19.23	120.22	110.60
22	BA	2860	A	N1-C6-N6	-19.23	107.06	118.60
1	AA	465	A	N1-C2-N3	-19.23	119.69	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	374	A	N1-C6-N6	-19.23	107.06	118.60
22	BA	347	A	N1-C6-N6	-19.23	107.06	118.60
22	BA	727	A	C2-N3-C4	19.23	120.21	110.60
22	BA	515	A	C2-N3-C4	19.22	120.21	110.60
22	BA	727	A	N1-C6-N6	-19.22	107.06	118.60
22	BA	190	A	N1-C6-N6	-19.22	107.07	118.60
1	AA	119	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	294	A	N1-C2-N3	-19.22	119.69	129.30
22	BA	1359	A	N1-C2-N3	-19.22	119.69	129.30
22	BA	1403	A	C2-N3-C4	19.22	120.21	110.60
1	AA	553	A	N1-C6-N6	-19.22	107.07	118.60
1	AA	1269	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	1272	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	602	A	C2-N3-C4	19.21	120.21	110.60
22	BA	2765	A	C2-N3-C4	19.21	120.21	110.60
23	BB	99	A	N1-C6-N6	-19.21	107.07	118.60
22	BA	899	A	N1-C6-N6	-19.21	107.08	118.60
22	BA	1020	A	N1-C2-N3	-19.21	119.70	129.30
22	BA	1936	A	N1-C6-N6	-19.21	107.08	118.60
55	B8	6	A	N1-C2-N3	-19.21	119.70	129.30
22	BA	1762	A	C2-N3-C4	19.21	120.20	110.60
22	BA	2266	A	N1-C6-N6	-19.21	107.08	118.60
22	BA	706	A	N1-C6-N6	-19.20	107.08	118.60
55	B8	42	A	N1-C6-N6	-19.20	107.08	118.60
22	BA	2577	A	N1-C6-N6	-19.20	107.08	118.60
1	AA	621	A	N1-C6-N6	-19.20	107.08	118.60
22	BA	74	A	N1-C6-N6	-19.20	107.08	118.60
1	AA	274	A	N1-C6-N6	-19.19	107.08	118.60
55	B8	76	A	N1-C2-N3	-19.19	119.70	129.30
22	BA	1504	A	N1-C6-N6	-19.19	107.09	118.60
22	BA	241	A	N1-C2-N3	-19.19	119.71	129.30
55	B8	58	A	C2-N3-C4	19.19	120.19	110.60
22	BA	1496	A	C2-N3-C4	19.19	120.19	110.60
22	BA	223	A	N1-C2-N3	-19.18	119.71	129.30
22	BA	1579	A	N1-C6-N6	-19.18	107.09	118.60
22	BA	2566	A	N1-C6-N6	-19.18	107.09	118.60
1	AA	583	A	N1-C6-N6	-19.18	107.09	118.60
22	BA	1570	A	N1-C2-N3	-19.18	119.71	129.30
1	AA	313	A	N1-C6-N6	-19.18	107.09	118.60
22	BA	2469	A	N1-C2-N3	-19.18	119.71	129.30
1	AA	872	A	N1-C6-N6	-19.17	107.10	118.60
22	BA	800	A	N1-C2-N3	-19.17	119.71	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2736	A	C2-N3-C4	19.17	120.19	110.60
22	BA	2101	A	N1-C6-N6	-19.17	107.10	118.60
22	BA	1254	A	N1-C6-N6	-19.17	107.10	118.60
22	BA	1739	A	C2-N3-C4	19.16	120.18	110.60
22	BA	2247	A	C2-N3-C4	19.16	120.18	110.60
22	BA	1544	A	N1-C2-N3	-19.16	119.72	129.30
22	BA	2059	A	N1-C6-N6	-19.16	107.11	118.60
22	BA	764	A	C2-N3-C4	19.16	120.18	110.60
22	BA	1626	A	N1-C2-N3	-19.16	119.72	129.30
22	BA	1383	A	N1-C6-N6	-19.16	107.11	118.60
22	BA	346	A	N1-C6-N6	-19.15	107.11	118.60
22	BA	877	A	N1-C6-N6	-19.15	107.11	118.60
22	BA	2005	A	N1-C2-N3	-19.15	119.72	129.30
1	AA	665	A	N1-C2-N3	-19.15	119.73	129.30
22	BA	199	A	C2-N3-C4	19.15	120.17	110.60
1	AA	179	A	N1-C6-N6	-19.15	107.11	118.60
22	BA	340	A	N1-C6-N6	-19.15	107.11	118.60
22	BA	793	A	N1-C2-N3	-19.14	119.73	129.30
22	BA	2134	A	N1-C6-N6	-19.14	107.11	118.60
22	BA	668	A	N1-C2-N3	-19.14	119.73	129.30
22	BA	222	A	C2-N3-C4	19.14	120.17	110.60
22	BA	2080	A	N1-C6-N6	-19.14	107.12	118.60
22	BA	2748	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	1327	A	N1-C6-N6	-19.13	107.12	118.60
22	BA	1378	A	C2-N3-C4	19.13	120.16	110.60
22	BA	1932	A	N1-C6-N6	-19.13	107.12	118.60
22	BA	2882	A	C2-N3-C4	19.13	120.16	110.60
1	AA	892	A	C2-N3-C4	19.12	120.16	110.60
55	B8	42	A	N1-C2-N3	-19.12	119.74	129.30
1	AA	60	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	541	A	C2-N3-C4	19.12	120.16	110.60
22	BA	1142	A	N1-C6-N6	-19.12	107.13	118.60
22	BA	1794	A	C2-N3-C4	19.12	120.16	110.60
22	BA	457	A	C2-N3-C4	19.12	120.16	110.60
22	BA	1848	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	2411	A	C2-N3-C4	19.12	120.16	110.60
22	BA	204	A	N1-C6-N6	-19.11	107.13	118.60
22	BA	789	A	N1-C6-N6	-19.11	107.13	118.60
22	BA	1453	A	N1-C6-N6	-19.11	107.13	118.60
22	BA	2054	A	C2-N3-C4	19.11	120.16	110.60
1	AA	816	A	C2-N3-C4	19.11	120.16	110.60
22	BA	1525	A	N1-C2-N3	-19.11	119.74	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	431	A	N1-C2-N3	-19.11	119.75	129.30
22	BA	439	A	C2-N3-C4	19.11	120.16	110.60
22	BA	2639	A	N1-C6-N6	-19.11	107.13	118.60
22	BA	2211	A	N1-C6-N6	-19.11	107.14	118.60
22	BA	219	A	C2-N3-C4	19.10	120.15	110.60
1	AA	1022	A	N1-C6-N6	-19.10	107.14	118.60
22	BA	2314	A	N1-C6-N6	-19.09	107.14	118.60
22	BA	2376	A	N1-C2-N3	-19.09	119.75	129.30
1	AA	1349	A	N1-C6-N6	-19.09	107.15	118.60
55	B8	73	A	N1-C2-N3	-19.09	119.76	129.30
1	AA	81	A	N1-C6-N6	-19.09	107.15	118.60
22	BA	1008	A	N1-C6-N6	-19.09	107.15	118.60
55	B8	51	A	N1-C2-N3	-19.09	119.76	129.30
22	BA	1342	A	N1-C6-N6	-19.08	107.15	118.60
22	BA	1156	A	C2-N3-C4	19.08	120.14	110.60
22	BA	2062	A	N1-C6-N6	-19.08	107.15	118.60
1	AA	1456	A	N1-C6-N6	-19.08	107.15	118.60
22	BA	984	A	C2-N3-C4	19.08	120.14	110.60
22	BA	2439	A	C2-N3-C4	19.08	120.14	110.60
22	BA	739	A	C2-N3-C4	19.07	120.14	110.60
22	BA	1490	A	N1-C6-N6	-19.07	107.16	118.60
1	AA	197	A	N1-C2-N3	-19.07	119.77	129.30
1	AA	1179	A	N1-C6-N6	-19.07	107.16	118.60
1	AA	1191	A	C2-N3-C4	19.07	120.14	110.60
22	BA	821	A	C2-N3-C4	19.07	120.14	110.60
1	AA	1513	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	2173	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	920	A	C2-N3-C4	19.07	120.13	110.60
1	AA	1333	A	C2-N3-C4	19.07	120.13	110.60
22	BA	94	A	N1-C6-N6	-19.06	107.16	118.60
22	BA	2003	A	N1-C6-N6	-19.06	107.16	118.60
1	AA	182	A	N1-C6-N6	-19.06	107.17	118.60
22	BA	899	A	C2-N3-C4	19.06	120.13	110.60
22	BA	2635	A	C2-N3-C4	19.05	120.13	110.60
22	BA	2738	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	1301	A	N1-C6-N6	-19.05	107.17	118.60
1	AA	787	A	N1-C2-N3	-19.05	119.77	129.30
22	BA	1901	A	N1-C6-N6	-19.05	107.17	118.60
1	AA	1188	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	1264	A	N1-C2-N3	-19.05	119.78	129.30
1	AA	715	A	C2-N3-C4	19.05	120.12	110.60
22	BA	2434	A	N1-C6-N6	-19.05	107.17	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	5	A	C2-N3-C4	19.04	120.12	110.60
22	BA	1204	A	N1-C2-N3	-19.04	119.78	129.30
22	BA	513	A	C2-N3-C4	19.04	120.12	110.60
22	BA	1698	A	N1-C6-N6	-19.04	107.18	118.60
22	BA	1265	A	C2-N3-C4	19.04	120.12	110.60
22	BA	2439	A	N1-C2-N3	-19.04	119.78	129.30
1	AA	7	A	N1-C6-N6	-19.03	107.18	118.60
22	BA	1395	A	N1-C2-N3	-19.03	119.78	129.30
22	BA	988	A	C2-N3-C4	19.03	120.12	110.60
22	BA	2070	A	C2-N3-C4	19.03	120.11	110.60
22	BA	1286	A	C2-N3-C4	19.03	120.11	110.60
22	BA	2051	A	C2-N3-C4	19.02	120.11	110.60
22	BA	1286	A	N1-C2-N3	-19.02	119.79	129.30
1	AA	336	A	N1-C6-N6	-19.02	107.19	118.60
1	AA	1476	A	C2-N3-C4	19.02	120.11	110.60
22	BA	1470	A	C2-N3-C4	19.02	120.11	110.60
22	BA	1932	A	N1-C2-N3	-19.02	119.79	129.30
1	AA	356	A	C2-N3-C4	19.02	120.11	110.60
22	BA	346	A	N1-C2-N3	-19.02	119.79	129.30
22	BA	1142	A	C2-N3-C4	19.02	120.11	110.60
22	BA	10	A	N1-C2-N3	-19.01	119.79	129.30
22	BA	609	A	N1-C6-N6	-19.01	107.19	118.60
22	BA	892	A	N1-C6-N6	-19.01	107.19	118.60
1	AA	539	A	C2-N3-C4	19.01	120.11	110.60
22	BA	941	A	C2-N3-C4	19.01	120.11	110.60
1	AA	712	A	C2-N3-C4	19.01	120.11	110.60
22	BA	819	A	C2-N3-C4	19.01	120.11	110.60
22	BA	1759	A	N1-C2-N3	-19.00	119.80	129.30
1	AA	313	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	2352	A	N1-C6-N6	-19.00	107.20	118.60
1	AA	975	A	N1-C6-N6	-19.00	107.20	118.60
55	B8	73	A	C2-N3-C4	19.00	120.10	110.60
22	BA	1175	A	N1-C6-N6	-18.99	107.20	118.60
22	BA	1495	A	N1-C6-N6	-18.99	107.21	118.60
22	BA	2468	A	N1-C2-N3	-18.99	119.81	129.30
22	BA	973	A	N1-C2-N3	-18.99	119.81	129.30
22	BA	2346	A	N1-C6-N6	-18.99	107.21	118.60
1	AA	1145	A	N1-C6-N6	-18.98	107.21	118.60
22	BA	1028	A	N1-C6-N6	-18.98	107.21	118.60
22	BA	1598	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	2267	A	C2-N3-C4	18.98	120.09	110.60
1	AA	1201	A	C2-N3-C4	18.98	120.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	815	A	N1-C6-N6	-18.98	107.21	118.60
22	BA	2311	A	N1-C6-N6	-18.98	107.21	118.60
22	BA	1815	A	N1-C2-N3	-18.98	119.81	129.30
1	AA	196	A	N1-C6-N6	-18.98	107.21	118.60
22	BA	2020	A	C2-N3-C4	18.98	120.09	110.60
22	BA	2406	A	C2-N3-C4	18.98	120.09	110.60
22	BA	111	A	C2-N3-C4	18.97	120.09	110.60
22	BA	1952	A	N1-C2-N3	-18.97	119.81	129.30
22	BA	2778	A	C2-N3-C4	18.97	120.09	110.60
22	BA	1809	A	N1-C2-N3	-18.97	119.82	129.30
22	BA	2298	A	N1-C6-N6	-18.97	107.22	118.60
22	BA	1244	A	N1-C2-N3	-18.97	119.82	129.30
22	BA	1981	A	N1-C6-N6	-18.97	107.22	118.60
22	BA	2453	A	N1-C6-N6	-18.97	107.22	118.60
22	BA	1616	A	N1-C6-N6	-18.96	107.22	118.60
1	AA	1499	A	N1-C6-N6	-18.96	107.22	118.60
22	BA	1144	A	C2-N3-C4	18.96	120.08	110.60
22	BA	2682	A	C2-N3-C4	18.96	120.08	110.60
22	BA	2212	A	N1-C2-N3	-18.96	119.82	129.30
1	AA	1434	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	91	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	804	A	N1-C2-N3	-18.95	119.82	129.30
1	AA	768	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	160	A	N1-C2-N3	-18.95	119.82	129.30
22	BA	231	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	627	A	N1-C2-N3	-18.95	119.82	129.30
1	AA	152	A	C2-N3-C4	18.95	120.08	110.60
22	BA	1569	A	C2-N3-C4	18.95	120.07	110.60
22	BA	2887	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	2734	A	C2-N3-C4	18.95	120.07	110.60
1	AA	1394	A	N1-C2-N3	-18.95	119.83	129.30
22	BA	925	A	C2-N3-C4	18.95	120.07	110.60
22	BA	1637	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	878	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	2090	A	C2-N3-C4	18.94	120.07	110.60
22	BA	2541	A	C2-N3-C4	18.94	120.07	110.60
1	AA	554	A	N1-C6-N6	-18.94	107.24	118.60
1	AA	673	A	N1-C6-N6	-18.94	107.24	118.60
1	AA	825	A	C2-N3-C4	18.94	120.07	110.60
22	BA	1549	A	C2-N3-C4	18.94	120.07	110.60
1	AA	414	A	N1-C6-N6	-18.94	107.24	118.60
22	BA	2451	A	N1-C2-N3	-18.94	119.83	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	675	A	N1-C6-N6	-18.94	107.24	118.60
22	BA	13	A	C2-N3-C4	18.94	120.07	110.60
22	BA	1477	A	N1-C2-N3	-18.94	119.83	129.30
1	AA	1340	A	C2-N3-C4	18.93	120.07	110.60
22	BA	943	A	C2-N3-C4	18.93	120.07	110.60
22	BA	2147	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	2850	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	127	A	N1-C2-N3	-18.93	119.84	129.30
1	AA	197	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	1385	A	N1-C6-N6	-18.93	107.25	118.60
22	BA	1937	A	C2-N3-C4	18.92	120.06	110.60
1	AA	977	A	C2-N3-C4	18.92	120.06	110.60
22	BA	402	A	N1-C6-N6	-18.92	107.25	118.60
1	AA	1016	A	N1-C6-N6	-18.92	107.25	118.60
22	BA	1548	A	C2-N3-C4	18.92	120.06	110.60
22	BA	608	A	N1-C6-N6	-18.92	107.25	118.60
22	BA	1593	A	C2-N3-C4	18.92	120.06	110.60
1	AA	32	A	C2-N3-C4	18.91	120.06	110.60
22	BA	432	A	C2-N3-C4	18.91	120.06	110.60
55	B8	41	A	C2-N3-C4	18.91	120.06	110.60
55	B8	73	A	N1-C6-N6	-18.91	107.25	118.60
1	AA	878	A	N1-C6-N6	-18.91	107.25	118.60
1	AA	1246	A	N1-C6-N6	-18.91	107.25	118.60
22	BA	819	A	N1-C6-N6	-18.91	107.25	118.60
22	BA	2564	A	C2-N3-C4	18.91	120.05	110.60
22	BA	2766	A	C2-N3-C4	18.91	120.05	110.60
1	AA	949	A	C2-N3-C4	18.91	120.05	110.60
22	BA	1571	A	C2-N3-C4	18.91	120.05	110.60
22	BA	1885	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	371	A	N1-C6-N6	-18.90	107.26	118.60
22	BA	861	A	C2-N3-C4	18.90	120.05	110.60
22	BA	2042	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	1571	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	265	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	1070	A	N1-C6-N6	-18.90	107.26	118.60
22	BA	1640	A	N1-C6-N6	-18.90	107.26	118.60
22	BA	1784	A	N1-C2-N3	-18.90	119.85	129.30
23	BB	29	A	N1-C6-N6	-18.90	107.26	118.60
1	AA	152	A	N1-C2-N3	-18.89	119.85	129.30
1	AA	1239	A	N1-C2-N3	-18.89	119.85	129.30
22	BA	643	A	N1-C2-N3	-18.89	119.85	129.30
22	BA	2590	A	C2-N3-C4	18.89	120.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2657	A	N1-C2-N3	-18.89	119.85	129.30
22	BA	2478	A	C2-N3-C4	18.89	120.05	110.60
22	BA	2518	A	C2-N3-C4	18.89	120.05	110.60
1	AA	116	A	N1-C6-N6	-18.89	107.27	118.60
22	BA	1127	A	N1-C6-N6	-18.89	107.27	118.60
22	BA	1213	A	C2-N3-C4	18.89	120.04	110.60
22	BA	2872	A	C5-C6-N6	18.88	138.81	123.70
1	AA	496	A	N1-C2-N3	-18.88	119.86	129.30
22	BA	1535	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	935	A	C2-N3-C4	18.88	120.04	110.60
22	BA	2340	A	N1-C2-N3	-18.88	119.86	129.30
22	BA	1155	A	N1-C2-N3	-18.88	119.86	129.30
22	BA	2459	A	C2-N3-C4	18.88	120.04	110.60
22	BA	332	A	N1-C2-N3	-18.88	119.86	129.30
1	AA	243	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	670	A	C2-N3-C4	18.87	120.04	110.60
1	AA	1248	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	802	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	972	A	N1-C2-N3	-18.87	119.86	129.30
1	AA	353	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	2119	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	501	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	507	A	C2-N3-C4	18.87	120.03	110.60
22	BA	165	A	C2-N3-C4	18.86	120.03	110.60
22	BA	310	A	C2-N3-C4	18.86	120.03	110.60
22	BA	453	A	C2-N3-C4	18.86	120.03	110.60
22	BA	1916	A	N1-C6-N6	-18.86	107.28	118.60
22	BA	2095	A	N1-C6-N6	-18.86	107.28	118.60
22	BA	1434	A	N1-C2-N3	-18.86	119.87	129.30
1	AA	353	A	C2-N3-C4	18.86	120.03	110.60
1	AA	1225	A	N1-C6-N6	-18.86	107.28	118.60
1	AA	1480	A	N1-C6-N6	-18.86	107.28	118.60
22	BA	415	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	637	A	C2-N3-C4	18.86	120.03	110.60
22	BA	735	A	C2-N3-C4	18.86	120.03	110.60
22	BA	1419	A	N1-C6-N6	-18.86	107.28	118.60
22	BA	2835	A	C2-N3-C4	18.86	120.03	110.60
22	BA	1001	A	C2-N3-C4	18.86	120.03	110.60
22	BA	1264	A	C2-N3-C4	18.86	120.03	110.60
22	BA	1744	A	N1-C6-N6	-18.86	107.28	118.60
22	BA	1640	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	265	A	C2-N3-C4	18.85	120.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1794	A	N1-C2-N3	-18.85	119.87	129.30
22	BA	2632	A	N1-C6-N6	-18.85	107.29	118.60
1	AA	622	A	N1-C2-N3	-18.85	119.87	129.30
1	AA	1019	A	N1-C6-N6	-18.85	107.29	118.60
1	AA	1110	A	N1-C6-N6	-18.85	107.29	118.60
22	BA	655	A	N1-C6-N6	-18.85	107.29	118.60
22	BA	515	A	N1-C2-N3	-18.85	119.88	129.30
22	BA	1901	A	C2-N3-C4	18.85	120.03	110.60
22	BA	479	A	C2-N3-C4	18.85	120.02	110.60
1	AA	949	A	N1-C6-N6	-18.84	107.29	118.60
22	BA	1803	A	N1-C2-N3	-18.84	119.88	129.30
22	BA	2823	A	N1-C2-N3	-18.84	119.88	129.30
22	BA	1551	A	C2-N3-C4	18.84	120.02	110.60
22	BA	2726	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	1238	A	C2-N3-C4	18.84	120.02	110.60
22	BA	64	A	C2-N3-C4	18.84	120.02	110.60
22	BA	231	A	C2-N3-C4	18.84	120.02	110.60
22	BA	1129	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	98	A	N1-C6-N6	-18.84	107.30	118.60
1	AA	573	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1363	A	C2-N3-C4	18.84	120.02	110.60
22	BA	508	A	N1-C2-N3	-18.83	119.88	129.30
22	BA	1359	A	N1-C6-N6	-18.83	107.30	118.60
1	AA	915	A	N1-C2-N3	-18.83	119.88	129.30
22	BA	1717	A	N1-C6-N6	-18.83	107.30	118.60
22	BA	699	A	C2-N3-C4	18.83	120.02	110.60
22	BA	2639	A	N1-C2-N3	-18.83	119.89	129.30
22	BA	1630	A	N1-C2-N3	-18.83	119.89	129.30
22	BA	1960	A	C2-N3-C4	18.83	120.01	110.60
1	AA	288	A	C2-N3-C4	18.83	120.01	110.60
1	AA	478	A	N1-C6-N6	-18.83	107.30	118.60
22	BA	217	A	C2-N3-C4	18.83	120.01	110.60
22	BA	1086	A	N1-C2-N3	-18.83	119.89	129.30
22	BA	1978	A	N1-C2-N3	-18.83	119.89	129.30
1	AA	1250	A	N1-C6-N6	-18.82	107.31	118.60
22	BA	2117	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	2173	A	C2-N3-C4	18.82	120.01	110.60
22	BA	2778	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	336	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	1978	A	C2-N3-C4	18.82	120.01	110.60
22	BA	2711	A	C2-N3-C4	18.82	120.01	110.60
22	BA	1237	A	N1-C2-N3	-18.82	119.89	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1791	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	913	A	N1-C2-N3	-18.81	119.89	129.30
22	BA	1322	A	N1-C6-N6	-18.81	107.31	118.60
22	BA	2516	A	C2-N3-C4	18.81	120.01	110.60
22	BA	1802	A	N1-C6-N6	-18.81	107.31	118.60
22	BA	1327	A	C2-N3-C4	18.81	120.00	110.60
22	BA	199	A	N1-C2-N3	-18.81	119.90	129.30
22	BA	265	A	N1-C6-N6	-18.81	107.31	118.60
22	BA	432	A	N1-C6-N6	-18.81	107.31	118.60
22	BA	990	A	C2-N3-C4	18.81	120.00	110.60
22	BA	1701	A	N1-C6-N6	-18.81	107.31	118.60
55	B8	51	A	C2-N3-C4	18.80	120.00	110.60
1	AA	364	A	N1-C6-N6	-18.80	107.32	118.60
22	BA	300	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	1759	A	N1-C6-N6	-18.80	107.32	118.60
22	BA	1772	A	N1-C6-N6	-18.80	107.32	118.60
23	BB	78	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1014	A	N1-C6-N6	-18.80	107.32	118.60
22	BA	422	A	C2-N3-C4	18.80	120.00	110.60
22	BA	1275	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	2426	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	2733	A	N1-C6-N6	-18.80	107.32	118.60
1	AA	596	A	C2-N3-C4	18.80	120.00	110.60
22	BA	42	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	661	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	1008	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	1342	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	1668	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	523	A	N1-C2-N3	-18.79	119.90	129.30
1	AA	1225	A	C2-N3-C4	18.79	119.99	110.60
22	BA	2268	A	N1-C6-N6	-18.79	107.33	118.60
1	AA	282	A	C2-N3-C4	18.79	119.99	110.60
1	AA	309	A	C2-N3-C4	18.79	119.99	110.60
22	BA	73	A	N1-C2-N3	-18.79	119.91	129.30
22	BA	582	A	C2-N3-C4	18.79	119.99	110.60
22	BA	2740	A	N1-C6-N6	-18.79	107.33	118.60
1	AA	459	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	1213	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	1428	A	C2-N3-C4	18.78	119.99	110.60
22	BA	432	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	2	A	C2-N3-C4	18.78	119.99	110.60
22	BA	429	A	N1-C2-N3	-18.78	119.91	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	563	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	2468	A	N1-C6-N6	-18.78	107.33	118.60
1	AA	238	A	N1-C6-N6	-18.77	107.34	118.60
1	AA	1035	A	C2-N3-C4	18.77	119.99	110.60
22	BA	255	A	C2-N3-C4	18.77	119.98	110.60
22	BA	689	A	N1-C6-N6	-18.77	107.34	118.60
22	BA	2471	A	N1-C2-N3	-18.77	119.92	129.30
23	BB	73	A	C2-N3-C4	18.77	119.98	110.60
22	BA	2433	A	N1-C2-N3	-18.77	119.92	129.30
1	AA	816	A	N1-C2-N3	-18.77	119.92	129.30
22	BA	1932	A	C2-N3-C4	18.76	119.98	110.60
22	BA	2094	A	N1-C6-N6	-18.76	107.34	118.60
22	BA	2602	A	N1-C6-N6	-18.76	107.34	118.60
23	BB	104	A	N1-C6-N6	-18.76	107.34	118.60
22	BA	1784	A	C2-N3-C4	18.76	119.98	110.60
22	BA	125	A	C2-N3-C4	18.76	119.98	110.60
22	BA	514	A	C2-N3-C4	18.76	119.98	110.60
22	BA	1194	A	C2-N3-C4	18.76	119.98	110.60
22	BA	1802	A	C2-N3-C4	18.76	119.98	110.60
55	B8	59	A	N1-C6-N6	-18.76	107.34	118.60
1	AA	120	A	N1-C2-N3	-18.76	119.92	129.30
22	BA	1048	A	N1-C6-N6	-18.76	107.35	118.60
22	BA	1395	A	C2-N3-C4	18.76	119.98	110.60
22	BA	1001	A	N1-C2-N3	-18.75	119.92	129.30
22	BA	1789	A	C2-N3-C4	18.75	119.98	110.60
22	BA	2635	A	N1-C6-N6	-18.75	107.35	118.60
1	AA	608	A	C2-N3-C4	18.75	119.98	110.60
22	BA	2761	A	N1-C6-N6	-18.75	107.35	118.60
22	BA	28	A	N1-C2-N3	-18.75	119.93	129.30
1	AA	1188	A	C2-N3-C4	18.75	119.97	110.60
22	BA	513	A	N1-C2-N3	-18.75	119.93	129.30
1	AA	572	A	N1-C2-N3	-18.75	119.93	129.30
1	AA	913	A	N1-C6-N6	-18.75	107.35	118.60
22	BA	2826	A	N1-C2-N3	-18.75	119.93	129.30
1	AA	655	A	C2-N3-C4	18.74	119.97	110.60
1	AA	675	A	C2-N3-C4	18.74	119.97	110.60
22	BA	1175	A	C2-N3-C4	18.74	119.97	110.60
1	AA	59	A	C2-N3-C4	18.74	119.97	110.60
22	BA	1597	A	C2-N3-C4	18.74	119.97	110.60
1	AA	502	A	C2-N3-C4	18.74	119.97	110.60
22	BA	1548	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	327	A	C2-N3-C4	18.74	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1189	A	N1-C6-N6	-18.74	107.36	118.60
1	AA	60	A	N1-C6-N6	-18.74	107.36	118.60
22	BA	2468	A	C2-N3-C4	18.74	119.97	110.60
22	BA	104	A	N1-C6-N6	-18.73	107.36	118.60
22	BA	460	A	C2-N3-C4	18.73	119.97	110.60
1	AA	694	A	C2-N3-C4	18.73	119.97	110.60
22	BA	1103	A	N1-C6-N6	-18.73	107.36	118.60
1	AA	1377	A	N1-C6-N6	-18.73	107.36	118.60
22	BA	1308	A	C2-N3-C4	18.73	119.96	110.60
22	BA	320	A	N1-C6-N6	-18.73	107.36	118.60
22	BA	1260	A	N1-C6-N6	-18.73	107.36	118.60
22	BA	2589	A	C2-N3-C4	18.73	119.96	110.60
22	BA	1069	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	2284	A	C2-N3-C4	18.72	119.96	110.60
22	BA	2471	A	C2-N3-C4	18.72	119.96	110.60
1	AA	573	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	1360	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	415	A	C2-N3-C4	18.72	119.96	110.60
22	BA	526	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	2054	A	N1-C2-N3	-18.72	119.94	129.30
22	BA	2327	A	N1-C2-N3	-18.72	119.94	129.30
22	BA	2274	A	N1-C6-N6	-18.71	107.37	118.60
22	BA	21	A	N1-C6-N6	-18.71	107.37	118.60
22	BA	1262	A	C2-N3-C4	18.71	119.95	110.60
22	BA	2450	A	C2-N3-C4	18.71	119.96	110.60
22	BA	2478	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	1044	A	N1-C6-N6	-18.71	107.38	118.60
22	BA	655	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	320	A	C2-N3-C4	18.71	119.95	110.60
22	BA	497	A	C2-N3-C4	18.70	119.95	110.60
22	BA	900	A	N1-C6-N6	-18.70	107.38	118.60
1	AA	1285	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	792	A	C2-N3-C4	18.70	119.95	110.60
23	BB	94	A	C2-N3-C4	18.70	119.95	110.60
22	BA	342	A	N1-C2-N3	-18.70	119.95	129.30
22	BA	347	A	C2-N3-C4	18.69	119.95	110.60
22	BA	1630	A	C2-N3-C4	18.69	119.95	110.60
22	BA	2560	A	N1-C6-N6	-18.69	107.39	118.60
1	AA	533	A	N1-C6-N6	-18.69	107.39	118.60
22	BA	14	A	C2-N3-C4	18.69	119.95	110.60
22	BA	693	A	C2-N3-C4	18.69	119.95	110.60
22	BA	1029	A	N1-C6-N6	-18.69	107.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1268	A	N1-C6-N6	-18.69	107.39	118.60
22	BA	176	A	C2-N3-C4	18.69	119.94	110.60
22	BA	255	A	N1-C2-N3	-18.69	119.96	129.30
22	BA	716	A	N1-C6-N6	-18.69	107.39	118.60
1	AA	382	A	C2-N3-C4	18.69	119.94	110.60
22	BA	1551	A	N1-C2-N3	-18.69	119.96	129.30
1	AA	1067	A	N1-C6-N6	-18.68	107.39	118.60
1	AA	1288	A	C2-N3-C4	18.68	119.94	110.60
22	BA	219	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	1048	A	C2-N3-C4	18.68	119.94	110.60
1	AA	533	A	C2-N3-C4	18.68	119.94	110.60
1	AA	969	A	N1-C6-N6	-18.68	107.39	118.60
22	BA	173	A	C2-N3-C4	18.68	119.94	110.60
22	BA	943	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	1230	A	C2-N3-C4	18.68	119.94	110.60
22	BA	454	A	N1-C6-N6	-18.68	107.39	118.60
1	AA	1332	A	C2-N3-C4	18.67	119.94	110.60
22	BA	905	A	C2-N3-C4	18.67	119.94	110.60
22	BA	2736	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	978	A	N1-C6-N6	-18.67	107.40	118.60
22	BA	1322	A	C2-N3-C4	18.67	119.94	110.60
23	BB	73	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	306	A	C2-N3-C4	18.67	119.93	110.60
1	AA	408	A	C2-N3-C4	18.67	119.93	110.60
22	BA	262	A	N1-C2-N3	-18.67	119.97	129.30
55	B8	21	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	1086	A	C2-N3-C4	18.66	119.93	110.60
22	BA	1285	A	C2-N3-C4	18.66	119.93	110.60
22	BA	1809	A	C2-N3-C4	18.66	119.93	110.60
22	BA	752	A	C2-N3-C4	18.66	119.93	110.60
22	BA	1977	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	1084	A	N1-C6-N6	-18.66	107.40	118.60
1	AA	263	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	172	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	1057	A	N1-C2-N3	-18.65	119.97	129.30
22	BA	1749	A	C2-N3-C4	18.65	119.93	110.60
1	AA	189	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	161	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	661	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	1151	A	C2-N3-C4	18.65	119.92	110.60
1	AA	412	A	C2-N3-C4	18.65	119.92	110.60
1	AA	1429	A	C2-N3-C4	18.65	119.92	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	84	A	C2-N3-C4	18.65	119.92	110.60
22	BA	789	A	C2-N3-C4	18.64	119.92	110.60
22	BA	2114	A	C2-N3-C4	18.64	119.92	110.60
22	BA	2700	A	N1-C6-N6	-18.64	107.41	118.60
1	AA	306	A	N1-C6-N6	-18.64	107.41	118.60
1	AA	1289	A	N1-C6-N6	-18.64	107.41	118.60
22	BA	125	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	2448	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	461	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1349	A	C2-N3-C4	18.64	119.92	110.60
1	AA	174	A	N1-C6-N6	-18.64	107.42	118.60
1	AA	1410	A	N1-C6-N6	-18.64	107.42	118.60
22	BA	959	A	N1-C6-N6	-18.64	107.42	118.60
22	BA	300	A	C2-N3-C4	18.64	119.92	110.60
22	BA	2448	A	C2-N3-C4	18.64	119.92	110.60
1	AA	101	A	C2-N3-C4	18.63	119.92	110.60
22	BA	675	A	N1-C2-N3	-18.63	119.98	129.30
22	BA	2879	A	C2-N3-C4	18.63	119.92	110.60
1	AA	1430	A	N1-C2-N3	-18.63	119.98	129.30
22	BA	1815	A	C2-N3-C4	18.63	119.92	110.60
22	BA	1439	A	N1-C2-N3	-18.63	119.98	129.30
22	BA	111	A	N1-C2-N3	-18.63	119.98	129.30
22	BA	1057	A	C2-N3-C4	18.63	119.91	110.60
22	BA	1384	A	C2-N3-C4	18.63	119.92	110.60
22	BA	1548	A	N1-C6-N6	-18.63	107.42	118.60
22	BA	74	A	C2-N3-C4	18.63	119.91	110.60
22	BA	2740	A	N1-C2-N3	-18.63	119.99	129.30
1	AA	1502	A	N1-C2-N3	-18.63	119.99	129.30
22	BA	391	A	N1-C2-N3	-18.63	119.99	129.30
22	BA	1393	A	N1-C2-N3	-18.63	119.99	129.30
22	BA	2835	A	N1-C2-N3	-18.63	119.99	129.30
1	AA	787	A	C2-N3-C4	18.62	119.91	110.60
1	AA	787	A	N1-C6-N6	-18.62	107.42	118.60
22	BA	1354	A	C2-N3-C4	18.62	119.91	110.60
22	BA	2142	A	C2-N3-C4	18.62	119.91	110.60
22	BA	49	A	N1-C6-N6	-18.62	107.43	118.60
22	BA	1264	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	393	A	C2-N3-C4	18.62	119.91	110.60
22	BA	42	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	1257	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	560	A	N1-C2-N3	-18.61	119.99	129.30
22	BA	1772	A	N1-C2-N3	-18.61	119.99	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	60	A	C2-N3-C4	18.61	119.91	110.60
1	AA	389	A	N1-C6-N6	-18.61	107.43	118.60
22	BA	1635	A	N1-C2-N3	-18.61	119.99	129.30
22	BA	2003	A	N1-C2-N3	-18.61	119.99	129.30
22	BA	2317	A	N1-C6-N6	-18.61	107.43	118.60
1	AA	174	A	C2-N3-C4	18.61	119.91	110.60
1	AA	26	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	918	A	C2-N3-C4	18.61	119.91	110.60
22	BA	429	A	C2-N3-C4	18.61	119.91	110.60
22	BA	10	A	C2-N3-C4	18.61	119.90	110.60
22	BA	94	A	C2-N3-C4	18.61	119.90	110.60
22	BA	2749	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	574	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	1780	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	1966	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	919	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	1046	A	C2-N3-C4	18.60	119.90	110.60
1	AA	766	A	C2-N3-C4	18.60	119.90	110.60
22	BA	750	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	197	A	C2-N3-C4	18.60	119.90	110.60
22	BA	820	A	N1-C6-N6	-18.60	107.44	118.60
22	BA	1321	A	N1-C6-N6	-18.60	107.44	118.60
22	BA	1739	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	1229	A	C2-N3-C4	18.60	119.90	110.60
22	BA	1672	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	547	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	1434	A	C2-N3-C4	18.59	119.90	110.60
1	AA	130	A	N1-C2-N3	-18.59	120.00	129.30
22	BA	794	A	N1-C2-N3	-18.59	120.00	129.30
22	BA	1899	A	N1-C6-N6	-18.59	107.44	118.60
1	AA	435	A	C2-N3-C4	18.59	119.89	110.60
22	BA	2392	A	C2-N3-C4	18.59	119.89	110.60
1	AA	1035	A	N1-C6-N6	-18.59	107.45	118.60
22	BA	1477	A	C2-N3-C4	18.59	119.89	110.60
22	BA	1754	A	C2-N3-C4	18.59	119.89	110.60
22	BA	1785	A	N1-C2-N3	-18.59	120.01	129.30
22	BA	2497	A	N1-C6-N6	-18.59	107.45	118.60
1	AA	1410	A	C2-N3-C4	18.59	119.89	110.60
22	BA	2665	A	C2-N3-C4	18.59	119.89	110.60
22	BA	1029	A	C2-N3-C4	18.59	119.89	110.60
1	AA	143	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	173	A	N1-C6-N6	-18.58	107.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	460	A	N1-C2-N3	-18.58	120.01	129.30
22	BA	2706	A	C2-N3-C4	18.58	119.89	110.60
22	BA	119	A	C2-N3-C4	18.58	119.89	110.60
1	AA	1285	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	51	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	1130	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	299	A	C2-N3-C4	18.58	119.89	110.60
23	BB	115	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	676	A	C2-N3-C4	18.58	119.89	110.60
1	AA	149	A	N1-C6-N6	-18.57	107.45	118.60
1	AA	1080	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	528	A	N1-C2-N3	-18.57	120.01	129.30
22	BA	1385	A	N1-C2-N3	-18.57	120.01	129.30
22	BA	1610	A	N1-C6-N6	-18.57	107.45	118.60
22	BA	244	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	1067	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	2598	A	C2-N3-C4	18.57	119.89	110.60
1	AA	389	A	C2-N3-C4	18.57	119.88	110.60
1	AA	435	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	294	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	1419	A	N1-C2-N3	-18.57	120.02	129.30
23	BB	50	A	C2-N3-C4	18.56	119.88	110.60
22	BA	2051	A	N1-C6-N6	-18.56	107.46	118.60
1	AA	1493	A	N1-C6-N6	-18.56	107.46	118.60
1	AA	1377	A	N1-C2-N3	-18.55	120.02	129.30
22	BA	1147	A	N1-C2-N3	-18.55	120.02	129.30
1	AA	1261	A	C2-N3-C4	18.55	119.88	110.60
22	BA	2856	A	C2-N3-C4	18.55	119.88	110.60
22	BA	1262	A	N1-C6-N6	-18.55	107.47	118.60
22	BA	1809	A	N1-C6-N6	-18.55	107.47	118.60
22	BA	2478	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	547	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	1157	A	C2-N3-C4	18.55	119.87	110.60
22	BA	845	A	C2-N3-C4	18.55	119.87	110.60
1	AA	1180	A	C2-N3-C4	18.55	119.87	110.60
22	BA	2309	A	N1-C6-N6	-18.55	107.47	118.60
55	B8	69	A	N1-C2-N3	-18.55	120.03	129.30
22	BA	2657	A	C2-N3-C4	18.54	119.87	110.60
1	AA	546	A	C2-N3-C4	18.54	119.87	110.60
1	AA	1152	A	C2-N3-C4	18.54	119.87	110.60
22	BA	146	A	C2-N3-C4	18.54	119.87	110.60
22	BA	508	A	C2-N3-C4	18.54	119.87	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	603	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1698	A	C2-N3-C4	18.54	119.87	110.60
1	AA	493	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1101	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1004	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	2392	A	N1-C6-N6	-18.54	107.48	118.60
1	AA	958	A	C2-N3-C4	18.54	119.87	110.60
1	AA	1499	A	C2-N3-C4	18.54	119.87	110.60
22	BA	404	A	N1-C6-N6	-18.54	107.48	118.60
22	BA	1650	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	1254	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1586	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1966	A	C2-N3-C4	18.54	119.87	110.60
22	BA	2392	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	596	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	866	A	N1-C2-N3	-18.53	120.03	129.30
22	BA	2738	A	C2-N3-C4	18.53	119.87	110.60
1	AA	131	A	C2-N3-C4	18.53	119.87	110.60
1	AA	802	A	C2-N3-C4	18.53	119.87	110.60
22	BA	1301	A	C2-N3-C4	18.53	119.87	110.60
1	AA	781	A	C2-N3-C4	18.53	119.86	110.60
1	AA	1252	A	C2-N3-C4	18.53	119.86	110.60
22	BA	28	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	1012	A	C2-N3-C4	18.53	119.86	110.60
1	AA	1289	A	N1-C2-N3	-18.53	120.04	129.30
22	BA	2823	A	C2-N3-C4	18.53	119.86	110.60
1	AA	595	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	1196	A	N1-C2-N3	-18.53	120.04	129.30
1	AA	466	A	C2-N3-C4	18.52	119.86	110.60
1	AA	909	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	1246	A	C2-N3-C4	18.52	119.86	110.60
22	BA	71	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	270	A	C2-N3-C4	18.52	119.86	110.60
22	BA	2062	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	2314	A	C2-N3-C4	18.52	119.86	110.60
22	BA	2761	A	C2-N3-C4	18.52	119.86	110.60
1	AA	72	A	C2-N3-C4	18.52	119.86	110.60
1	AA	914	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	1284	A	N1-C6-N6	-18.52	107.49	118.60
22	BA	1525	A	C2-N3-C4	18.52	119.86	110.60
22	BA	2450	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	116	A	N1-C2-N3	-18.52	120.04	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	696	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	1036	A	C2-N3-C4	18.52	119.86	110.60
22	BA	1805	A	C2-N3-C4	18.52	119.86	110.60
22	BA	2776	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	348	A	C2-N3-C4	18.52	119.86	110.60
22	BA	644	A	C2-N3-C4	18.52	119.86	110.60
1	AA	306	A	N1-C2-N3	-18.51	120.04	129.30
1	AA	460	A	N1-C2-N3	-18.51	120.04	129.30
1	AA	892	A	N1-C6-N6	-18.51	107.49	118.60
22	BA	502	A	N1-C2-N3	-18.51	120.04	129.30
22	BA	1808	A	C2-N3-C4	18.51	119.86	110.60
22	BA	742	A	C2-N3-C4	18.51	119.85	110.60
22	BA	756	A	C2-N3-C4	18.51	119.86	110.60
1	AA	728	A	C2-N3-C4	18.51	119.85	110.60
1	AA	983	A	C2-N3-C4	18.51	119.85	110.60
1	AA	1280	A	N1-C6-N6	-18.51	107.50	118.60
22	BA	793	A	C2-N3-C4	18.51	119.85	110.60
22	BA	2088	A	C2-N3-C4	18.51	119.85	110.60
1	AA	161	A	N1-C6-N6	-18.51	107.50	118.60
22	BA	190	A	C2-N3-C4	18.51	119.85	110.60
1	AA	327	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	393	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	2829	A	C2-N3-C4	18.50	119.85	110.60
23	BB	109	A	C2-N3-C4	18.50	119.85	110.60
22	BA	1144	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	1070	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	2765	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	1008	A	C2-N3-C4	18.50	119.85	110.60
1	AA	946	A	C2-N3-C4	18.50	119.85	110.60
22	BA	670	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	981	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	1365	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	2134	A	C2-N3-C4	18.50	119.85	110.60
23	BB	58	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	899	A	N1-C2-N3	-18.49	120.05	129.30
22	BA	1635	A	C2-N3-C4	18.49	119.85	110.60
22	BA	1927	A	C2-N3-C4	18.49	119.85	110.60
22	BA	2154	A	C2-N3-C4	18.49	119.85	110.60
22	BA	1785	A	N1-C6-N6	-18.49	107.50	118.60
22	BA	299	A	N1-C2-N3	-18.49	120.06	129.30
22	BA	943	A	N1-C6-N6	-18.49	107.51	118.60
22	BA	1626	A	C2-N3-C4	18.49	119.84	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2778	A	N1-C6-N6	-18.49	107.51	118.60
1	AA	1368	A	C2-N3-C4	18.49	119.84	110.60
1	AA	509	A	N1-C6-N6	-18.49	107.51	118.60
22	BA	2191	A	N1-C6-N6	-18.49	107.51	118.60
22	BA	2377	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	189	A	C2-N3-C4	18.48	119.84	110.60
1	AA	959	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	1101	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	1634	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	2311	A	C2-N3-C4	18.48	119.84	110.60
22	BA	2322	A	C2-N3-C4	18.48	119.84	110.60
1	AA	1080	A	N1-C2-N3	-18.48	120.06	129.30
23	BB	104	A	C2-N3-C4	18.48	119.84	110.60
1	AA	1318	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	983	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	167	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	928	A	C2-N3-C4	18.48	119.84	110.60
22	BA	1204	A	C2-N3-C4	18.48	119.84	110.60
22	BA	2560	A	C2-N3-C4	18.48	119.84	110.60
22	BA	1009	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	1762	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	2850	A	C2-N3-C4	18.48	119.84	110.60
23	BB	39	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	715	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	221	A	N1-C6-N6	-18.48	107.52	118.60
22	BA	1583	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	665	A	C2-N3-C4	18.47	119.84	110.60
23	BB	104	A	N1-C2-N3	-18.47	120.06	129.30
1	AA	964	A	C2-N3-C4	18.47	119.83	110.60
22	BA	1384	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	349	A	C2-N3-C4	18.47	119.83	110.60
1	AA	1067	A	N1-C2-N3	-18.47	120.07	129.30
22	BA	933	A	C2-N3-C4	18.46	119.83	110.60
22	BA	2126	A	N1-C6-N6	-18.46	107.52	118.60
22	BA	2518	A	N1-C6-N6	-18.46	107.52	118.60
55	B8	69	A	N1-C6-N6	-18.46	107.52	118.60
1	AA	1005	A	C2-N3-C4	18.46	119.83	110.60
22	BA	1274	A	C2-N3-C4	18.46	119.83	110.60
22	BA	2070	A	N1-C2-N3	-18.46	120.07	129.30
55	B8	58	A	N1-C6-N6	-18.46	107.52	118.60
1	AA	622	A	C2-N3-C4	18.46	119.83	110.60
1	AA	753	A	N1-C2-N3	-18.46	120.07	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1105	A	C2-N3-C4	18.46	119.83	110.60
1	AA	1145	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	21	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	2317	A	C2-N3-C4	18.46	119.83	110.60
1	AA	878	A	C2-N3-C4	18.46	119.83	110.60
1	AA	1311	A	C2-N3-C4	18.46	119.83	110.60
22	BA	127	A	N1-C6-N6	-18.46	107.52	118.60
22	BA	165	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	453	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	2270	A	N1-C6-N6	-18.46	107.53	118.60
22	BA	53	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	1717	A	C2-N3-C4	18.45	119.83	110.60
23	BB	45	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	2705	A	C2-N3-C4	18.45	119.83	110.60
22	BA	825	A	N1-C2-N3	-18.45	120.08	129.30
22	BA	1593	A	N1-C2-N3	-18.45	120.08	129.30
1	AA	889	A	N1-C2-N3	-18.45	120.08	129.30
54	B7	9	A	N1-C2-N3	-18.45	120.08	129.30
22	BA	279	A	N1-C2-N3	-18.45	120.08	129.30
22	BA	2757	A	C2-N3-C4	18.45	119.82	110.60
22	BA	1427	A	C2-N3-C4	18.45	119.82	110.60
22	BA	2810	A	C2-N3-C4	18.45	119.82	110.60
22	BA	1593	A	N1-C6-N6	-18.44	107.53	118.60
1	AA	262	A	N1-C2-N3	-18.44	120.08	129.30
22	BA	279	A	C2-N3-C4	18.44	119.82	110.60
22	BA	382	A	C2-N3-C4	18.44	119.82	110.60
22	BA	1069	A	N1-C2-N3	-18.44	120.08	129.30
22	BA	1745	A	N1-C2-N3	-18.44	120.08	129.30
1	AA	1042	A	N1-C6-N6	-18.43	107.54	118.60
55	B8	66	A	C2-N3-C4	18.43	119.82	110.60
1	AA	262	A	C2-N3-C4	18.43	119.82	110.60
1	AA	675	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	746	A	C2-N3-C4	18.43	119.82	110.60
22	BA	1039	A	N1-C6-N6	-18.43	107.54	118.60
22	BA	2809	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	160	A	N1-C2-N3	-18.43	120.08	129.30
22	BA	1786	A	N1-C2-N3	-18.43	120.09	129.30
22	BA	2572	A	C2-N3-C4	18.43	119.81	110.60
1	AA	349	A	N1-C6-N6	-18.43	107.54	118.60
22	BA	1046	A	N1-C6-N6	-18.43	107.54	118.60
22	BA	204	A	C2-N3-C4	18.43	119.81	110.60
22	BA	781	A	C2-N3-C4	18.43	119.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1288	A	N1-C6-N6	-18.42	107.55	118.60
1	AA	938	A	N1-C6-N6	-18.42	107.55	118.60
1	AA	1204	A	N1-C6-N6	-18.42	107.55	118.60
22	BA	2887	A	C2-N3-C4	18.42	119.81	110.60
22	BA	2366	A	C2-N3-C4	18.42	119.81	110.60
22	BA	2426	A	C2-N3-C4	18.42	119.81	110.60
22	BA	2461	A	C2-N3-C4	18.42	119.81	110.60
23	BB	108	A	N1-C2-N3	-18.42	120.09	129.30
1	AA	1016	A	C2-N3-C4	18.42	119.81	110.60
1	AA	411	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	910	A	C2-N3-C4	18.42	119.81	110.60
22	BA	2734	A	N1-C2-N3	-18.42	120.09	129.30
1	AA	977	A	N1-C6-N6	-18.42	107.55	118.60
22	BA	2287	A	N1-C2-N3	-18.42	120.09	129.30
1	AA	906	A	C2-N3-C4	18.41	119.81	110.60
1	AA	640	A	C2-N3-C4	18.41	119.81	110.60
22	BA	1918	A	N1-C6-N6	-18.41	107.55	118.60
1	AA	53	A	C2-N3-C4	18.41	119.81	110.60
1	AA	349	A	N1-C2-N3	-18.41	120.09	129.30
1	AA	510	A	N1-C2-N3	-18.41	120.09	129.30
1	AA	1044	A	C2-N3-C4	18.41	119.81	110.60
22	BA	1549	A	N1-C6-N6	-18.41	107.55	118.60
22	BA	278	A	N1-C2-N3	-18.41	120.09	129.30
1	AA	560	A	C2-N3-C4	18.41	119.80	110.60
1	AA	1169	A	N1-C6-N6	-18.41	107.56	118.60
22	BA	2288	A	N1-C2-N3	-18.41	120.10	129.30
1	AA	1319	A	N1-C6-N6	-18.41	107.56	118.60
22	BA	294	A	C2-N3-C4	18.41	119.80	110.60
22	BA	1700	A	N1-C6-N6	-18.41	107.56	118.60
22	BA	1783	A	C2-N3-C4	18.41	119.80	110.60
1	AA	315	A	N1-C6-N6	-18.41	107.56	118.60
22	BA	2764	A	N1-C2-N3	-18.41	120.10	129.30
22	BA	1821	A	C2-N3-C4	18.40	119.80	110.60
22	BA	2899	A	N1-C6-N6	-18.40	107.56	118.60
22	BA	2042	A	C2-N3-C4	18.40	119.80	110.60
22	BA	2893	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	825	A	N1-C2-N3	-18.40	120.10	129.30
22	BA	829	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	1319	A	N1-C2-N3	-18.40	120.10	129.30
22	BA	2015	A	C2-N3-C4	18.40	119.80	110.60
22	BA	2062	A	C2-N3-C4	18.40	119.80	110.60
22	BA	590	A	N1-C6-N6	-18.39	107.56	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	706	A	C2-N3-C4	18.39	119.80	110.60
22	BA	44	A	N1-C6-N6	-18.39	107.56	118.60
22	BA	2860	A	N1-C2-N3	-18.39	120.10	129.30
22	BA	492	A	N1-C2-N3	-18.39	120.11	129.30
22	BA	613	A	C2-N3-C4	18.39	119.80	110.60
22	BA	972	A	N1-C6-N6	-18.39	107.57	118.60
22	BA	1403	A	N1-C6-N6	-18.39	107.57	118.60
1	AA	908	A	N1-C6-N6	-18.39	107.57	118.60
22	BA	2632	A	C2-N3-C4	18.39	119.80	110.60
55	B8	6	A	N1-C6-N6	-18.39	107.57	118.60
1	AA	246	A	N1-C2-N3	-18.39	120.11	129.30
1	AA	1329	A	N1-C6-N6	-18.39	107.57	118.60
22	BA	2799	A	C2-N3-C4	18.39	119.79	110.60
1	AA	1329	A	C2-N3-C4	18.39	119.79	110.60
22	BA	172	A	C2-N3-C4	18.39	119.79	110.60
22	BA	670	A	N1-C2-N3	-18.39	120.11	129.30
22	BA	322	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	777	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	2376	A	C2-N3-C4	18.38	119.79	110.60
22	BA	2598	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	2516	A	N1-C6-N6	-18.38	107.57	118.60
1	AA	1499	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	196	A	C2-N3-C4	18.38	119.79	110.60
1	AA	236	A	N1-C6-N6	-18.38	107.57	118.60
1	AA	243	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	1251	A	N1-C6-N6	-18.38	107.57	118.60
1	AA	1261	A	N1-C6-N6	-18.38	107.57	118.60
1	AA	1350	A	C2-N3-C4	18.38	119.79	110.60
22	BA	429	A	N1-C6-N6	-18.38	107.58	118.60
22	BA	497	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	945	A	N1-C6-N6	-18.38	107.57	118.60
22	BA	1808	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	1918	A	C2-N3-C4	18.37	119.79	110.60
22	BA	1969	A	N1-C2-N3	-18.37	120.11	129.30
22	BA	789	A	N1-C2-N3	-18.37	120.11	129.30
22	BA	1803	A	C2-N3-C4	18.37	119.79	110.60
22	BA	1858	A	C2-N3-C4	18.37	119.79	110.60
1	AA	288	A	N1-C2-N3	-18.37	120.11	129.30
1	AA	1005	A	N1-C6-N6	-18.37	107.58	118.60
22	BA	492	A	N1-C6-N6	-18.37	107.58	118.60
1	AA	8	A	N1-C2-N3	-18.37	120.12	129.30
1	AA	676	A	N1-C2-N3	-18.37	120.12	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1155	A	C2-N3-C4	18.37	119.78	110.60
1	AA	573	A	N1-C6-N6	-18.37	107.58	118.60
22	BA	2199	A	N1-C2-N3	-18.37	120.12	129.30
22	BA	2114	A	N1-C6-N6	-18.36	107.58	118.60
22	BA	905	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	1885	A	N1-C6-N6	-18.36	107.58	118.60
22	BA	2873	A	N1-C2-N3	-18.36	120.12	129.30
1	AA	1413	A	N1-C6-N6	-18.36	107.58	118.60
22	BA	401	A	C2-N3-C4	18.36	119.78	110.60
22	BA	735	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	2565	A	N1-C2-N3	-18.36	120.12	129.30
1	AA	344	A	N1-C6-N6	-18.36	107.58	118.60
22	BA	508	A	N1-C6-N6	-18.36	107.58	118.60
22	BA	592	A	N1-C6-N6	-18.36	107.58	118.60
22	BA	2377	A	C2-N3-C4	18.36	119.78	110.60
22	BA	2632	A	N1-C2-N3	-18.36	120.12	129.30
1	AA	1362	A	N1-C6-N6	-18.36	107.59	118.60
22	BA	1596	A	N1-C6-N6	-18.36	107.59	118.60
22	BA	2453	A	N1-C2-N3	-18.36	120.12	129.30
1	AA	2	A	N1-C6-N6	-18.36	107.59	118.60
22	BA	423	A	N1-C2-N3	-18.35	120.12	129.30
1	AA	532	A	C2-N3-C4	18.35	119.78	110.60
22	BA	1067	A	N1-C2-N3	-18.35	120.12	129.30
22	BA	1885	A	C2-N3-C4	18.35	119.78	110.60
22	BA	2377	A	N1-C6-N6	-18.35	107.59	118.60
22	BA	256	A	C2-N3-C4	18.35	119.77	110.60
22	BA	1067	A	C2-N3-C4	18.35	119.77	110.60
22	BA	1085	A	C2-N3-C4	18.35	119.77	110.60
1	AA	1110	A	C2-N3-C4	18.35	119.77	110.60
22	BA	74	A	N1-C2-N3	-18.35	120.13	129.30
22	BA	800	A	C2-N3-C4	18.35	119.77	110.60
22	BA	103	A	N1-C6-N6	-18.34	107.59	118.60
1	AA	1150	A	N1-C6-N6	-18.34	107.59	118.60
55	B8	26	A	C2-N3-C4	18.34	119.77	110.60
1	AA	8	A	N1-C6-N6	-18.34	107.60	118.60
1	AA	26	A	C2-N3-C4	18.34	119.77	110.60
1	AA	1324	A	C2-N3-C4	18.34	119.77	110.60
23	BB	99	A	C2-N3-C4	18.34	119.77	110.60
1	AA	1289	A	C2-N3-C4	18.33	119.77	110.60
22	BA	195	A	N1-C2-N3	-18.33	120.13	129.30
22	BA	502	A	C2-N3-C4	18.33	119.77	110.60
1	AA	72	A	N1-C2-N3	-18.33	120.13	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	448	A	N1-C6-N6	-18.33	107.60	118.60
1	AA	1333	A	N1-C2-N3	-18.33	120.13	129.30
22	BA	556	A	C2-N3-C4	18.33	119.77	110.60
22	BA	2376	A	N1-C6-N6	-18.33	107.60	118.60
1	AA	393	A	N1-C6-N6	-18.33	107.60	118.60
1	AA	1081	A	C2-N3-C4	18.33	119.77	110.60
1	AA	1117	A	N1-C2-N3	-18.33	120.14	129.30
22	BA	447	A	N1-C2-N3	-18.33	120.14	129.30
22	BA	1057	A	N1-C6-N6	-18.33	107.60	118.60
22	BA	2565	A	C2-N3-C4	18.33	119.77	110.60
22	BA	2750	A	N1-C2-N3	-18.33	120.14	129.30
22	BA	877	A	C2-N3-C4	18.33	119.76	110.60
54	B7	9	A	N1-C6-N6	-18.33	107.60	118.60
22	BA	447	A	N1-C6-N6	-18.33	107.61	118.60
22	BA	892	A	C2-N3-C4	18.32	119.76	110.60
22	BA	227	A	C2-N3-C4	18.32	119.76	110.60
1	AA	753	A	C2-N3-C4	18.32	119.76	110.60
22	BA	332	A	C2-N3-C4	18.32	119.76	110.60
22	BA	863	A	C2-N3-C4	18.32	119.76	110.60
1	AA	1036	A	N1-C6-N6	-18.32	107.61	118.60
22	BA	866	A	C2-N3-C4	18.32	119.76	110.60
1	AA	182	A	N1-C2-N3	-18.32	120.14	129.30
22	BA	1900	A	C2-N3-C4	18.32	119.76	110.60
23	BB	115	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	1377	A	C2-N3-C4	18.32	119.76	110.60
22	BA	742	A	N1-C2-N3	-18.32	120.14	129.30
22	BA	984	A	N1-C2-N3	-18.32	120.14	129.30
22	BA	1566	A	N1-C2-N3	-18.31	120.14	129.30
1	AA	174	A	N1-C2-N3	-18.31	120.14	129.30
22	BA	990	A	N1-C2-N3	-18.31	120.14	129.30
22	BA	1420	A	C2-N3-C4	18.31	119.76	110.60
22	BA	2564	A	N1-C6-N6	-18.31	107.61	118.60
1	AA	81	A	C2-N3-C4	18.31	119.75	110.60
22	BA	1085	A	N1-C6-N6	-18.31	107.62	118.60
1	AA	814	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	2205	A	C2-N3-C4	18.30	119.75	110.60
22	BA	928	A	N1-C6-N6	-18.30	107.62	118.60
55	B8	51	A	N1-C6-N6	-18.30	107.62	118.60
1	AA	74	A	N1-C6-N6	-18.30	107.62	118.60
1	AA	344	A	N1-C2-N3	-18.30	120.15	129.30
22	BA	1773	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	368	A	N1-C6-N6	-18.30	107.62	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2184	A	N1-C6-N6	-18.30	107.62	118.60
1	AA	496	A	C2-N3-C4	18.30	119.75	110.60
22	BA	2198	A	C2-N3-C4	18.30	119.75	110.60
22	BA	2278	A	C2-N3-C4	18.30	119.75	110.60
1	AA	974	A	N1-C2-N3	-18.30	120.15	129.30
1	AA	1171	A	C2-N3-C4	18.30	119.75	110.60
22	BA	2566	A	C2-N3-C4	18.29	119.75	110.60
1	AA	546	A	N1-C6-N6	-18.29	107.62	118.60
22	BA	1877	A	N1-C6-N6	-18.29	107.62	118.60
1	AA	131	A	N1-C6-N6	-18.29	107.62	118.60
1	AA	1080	A	C2-N3-C4	18.29	119.75	110.60
22	BA	2639	A	C2-N3-C4	18.29	119.75	110.60
22	BA	804	A	C2-N3-C4	18.29	119.75	110.60
22	BA	1354	A	N1-C2-N3	-18.29	120.16	129.30
22	BA	749	A	N1-C6-N6	-18.29	107.63	118.60
22	BA	927	A	C2-N3-C4	18.29	119.74	110.60
22	BA	103	A	C2-N3-C4	18.29	119.74	110.60
22	BA	278	A	N1-C6-N6	-18.29	107.63	118.60
22	BA	1129	A	C2-N3-C4	18.29	119.74	110.60
22	BA	2471	A	N1-C6-N6	-18.29	107.63	118.60
1	AA	98	A	C2-N3-C4	18.29	119.74	110.60
22	BA	541	A	N1-C2-N3	-18.29	120.16	129.30
22	BA	1889	A	C2-N3-C4	18.28	119.74	110.60
1	AA	1447	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	1679	A	N1-C6-N6	-18.28	107.63	118.60
22	BA	2476	A	C2-N3-C4	18.28	119.74	110.60
1	AA	635	A	C2-N3-C4	18.28	119.74	110.60
1	AA	236	A	C2-N3-C4	18.28	119.74	110.60
1	AA	315	A	C2-N3-C4	18.28	119.74	110.60
1	AA	767	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	644	A	N1-C6-N6	-18.28	107.63	118.60
22	BA	1077	A	N1-C6-N6	-18.28	107.63	118.60
1	AA	1	A	C2-N3-C4	18.27	119.74	110.60
1	AA	482	A	C2-N3-C4	18.27	119.74	110.60
1	AA	608	A	N1-C2-N3	-18.27	120.16	129.30
22	BA	64	A	N1-C6-N6	-18.27	107.64	118.60
1	AA	909	A	C2-N3-C4	18.27	119.73	110.60
1	AA	1329	A	N1-C2-N3	-18.27	120.16	129.30
1	AA	1430	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	1665	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	633	A	N1-C6-N6	-18.27	107.64	118.60
1	AA	456	A	N1-C2-N3	-18.27	120.17	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	14	A	N1-C2-N3	-18.27	120.17	129.30
22	BA	1090	A	N1-C6-N6	-18.27	107.64	118.60
1	AA	579	A	C2-N3-C4	18.27	119.73	110.60
22	BA	2015	A	N1-C2-N3	-18.27	120.17	129.30
22	BA	2163	A	N1-C6-N6	-18.27	107.64	118.60
1	AA	539	A	N1-C6-N6	-18.26	107.64	118.60
22	BA	2547	A	C2-N3-C4	18.26	119.73	110.60
1	AA	374	A	C2-N3-C4	18.26	119.73	110.60
22	BA	541	A	N1-C6-N6	-18.26	107.64	118.60
22	BA	1090	A	N1-C2-N3	-18.26	120.17	129.30
1	AA	1251	A	C2-N3-C4	18.26	119.73	110.60
22	BA	1597	A	N1-C2-N3	-18.26	120.17	129.30
55	B8	69	A	C2-N3-C4	18.26	119.73	110.60
1	AA	1	A	N1-C6-N6	-18.26	107.65	118.60
22	BA	988	A	N1-C2-N3	-18.26	120.17	129.30
22	BA	1143	A	N1-C2-N3	-18.25	120.17	129.30
22	BA	1503	A	N1-C2-N3	-18.25	120.17	129.30
22	BA	2749	A	C2-N3-C4	18.25	119.73	110.60
1	AA	1269	A	C2-N3-C4	18.25	119.72	110.60
22	BA	44	A	C2-N3-C4	18.25	119.73	110.60
22	BA	466	A	C2-N3-C4	18.25	119.73	110.60
22	BA	877	A	N1-C2-N3	-18.25	120.17	129.30
1	AA	1042	A	C2-N3-C4	18.25	119.72	110.60
22	BA	241	A	C2-N3-C4	18.25	119.72	110.60
22	BA	2171	A	N1-C2-N3	-18.25	120.17	129.30
1	AA	802	A	N1-C2-N3	-18.25	120.18	129.30
1	AA	1021	A	N1-C2-N3	-18.25	120.18	129.30
22	BA	480	A	C2-N3-C4	18.25	119.72	110.60
22	BA	2792	A	C2-N3-C4	18.25	119.72	110.60
1	AA	493	A	N1-C6-N6	-18.25	107.65	118.60
1	AA	622	A	N1-C6-N6	-18.25	107.65	118.60
1	AA	919	A	C2-N3-C4	18.25	119.72	110.60
22	BA	1127	A	N1-C2-N3	-18.25	120.18	129.30
22	BA	1262	A	N1-C2-N3	-18.25	120.18	129.30
1	AA	53	A	N1-C2-N3	-18.24	120.18	129.30
1	AA	767	A	C2-N3-C4	18.24	119.72	110.60
22	BA	1050	A	N1-C6-N6	-18.24	107.65	118.60
22	BA	2887	A	N1-C2-N3	-18.24	120.18	129.30
1	AA	172	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	586	A	C2-N3-C4	18.24	119.72	110.60
22	BA	910	A	N1-C6-N6	-18.24	107.66	118.60
22	BA	1509	A	C2-N3-C4	18.24	119.72	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1700	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	2117	A	N1-C6-N6	-18.24	107.66	118.60
1	AA	1093	A	C2-N3-C4	18.24	119.72	110.60
22	BA	1654	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	1713	A	N1-C2-N3	-18.24	120.18	129.30
1	AA	1229	A	N1-C6-N6	-18.24	107.66	118.60
22	BA	1495	A	C2-N3-C4	18.24	119.72	110.60
22	BA	2589	A	N1-C2-N3	-18.24	120.18	129.30
1	AA	1105	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	146	A	N1-C6-N6	-18.23	107.66	118.60
22	BA	244	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	783	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	1569	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	1928	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	2590	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	2531	A	N1-C6-N6	-18.23	107.66	118.60
1	AA	7	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	2872	A	N1-C2-N3	-18.23	120.18	129.30
1	AA	1362	A	C2-N3-C4	18.23	119.72	110.60
22	BA	203	A	C2-N3-C4	18.23	119.72	110.60
1	AA	547	A	N1-C2-N3	-18.23	120.19	129.30
22	BA	1580	A	N1-C6-N6	-18.23	107.66	118.60
1	AA	353	A	N1-C2-N3	-18.23	120.19	129.30
22	BA	739	A	N1-C6-N6	-18.23	107.67	118.60
22	BA	829	A	N1-C6-N6	-18.23	107.67	118.60
22	BA	1522	A	C2-N3-C4	18.23	119.71	110.60
1	AA	171	A	N1-C2-N3	-18.22	120.19	129.30
22	BA	599	A	N1-C2-N3	-18.22	120.19	129.30
22	BA	1504	A	C2-N3-C4	18.22	119.71	110.60
1	AA	499	A	N1-C6-N6	-18.22	107.67	118.60
55	B8	59	A	C2-N3-C4	18.22	119.71	110.60
1	AA	1022	A	C2-N3-C4	18.22	119.71	110.60
22	BA	1085	A	N1-C2-N3	-18.22	120.19	129.30
22	BA	1490	A	C2-N3-C4	18.22	119.71	110.60
22	BA	1515	A	N1-C2-N3	-18.22	120.19	129.30
22	BA	1522	A	N1-C2-N3	-18.22	120.19	129.30
22	BA	1928	A	N1-C6-N6	-18.22	107.67	118.60
1	AA	1269	A	N1-C2-N3	-18.21	120.19	129.30
22	BA	705	A	C2-N3-C4	18.21	119.71	110.60
22	BA	1226	A	N1-C6-N6	-18.21	107.67	118.60
22	BA	1916	A	C2-N3-C4	18.21	119.71	110.60
22	BA	2411	A	N1-C2-N3	-18.21	120.19	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	412	A	N1-C2-N3	-18.21	120.19	129.30
22	BA	2856	A	N1-C6-N6	-18.21	107.67	118.60
22	BA	430	A	N1-C2-N3	-18.21	120.19	129.30
22	BA	1070	A	C2-N3-C4	18.21	119.70	110.60
22	BA	2298	A	C2-N3-C4	18.21	119.70	110.60
22	BA	118	A	C2-N3-C4	18.21	119.70	110.60
22	BA	2821	A	C2-N3-C4	18.21	119.70	110.60
22	BA	1469	A	C2-N3-C4	18.20	119.70	110.60
1	AA	600	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	1143	A	C2-N3-C4	18.20	119.70	110.60
1	AA	120	A	C2-N3-C4	18.20	119.70	110.60
1	AA	303	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	2634	A	N1-C6-N6	-18.20	107.68	118.60
1	AA	238	A	C2-N3-C4	18.20	119.70	110.60
1	AA	889	A	C2-N3-C4	18.20	119.70	110.60
22	BA	1096	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	1272	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	716	A	C2-N3-C4	18.20	119.70	110.60
23	BB	29	A	C2-N3-C4	18.20	119.70	110.60
1	AA	958	A	N1-C2-N3	-18.19	120.20	129.30
22	BA	1089	A	N1-C6-N6	-18.19	107.68	118.60
55	B8	38	A	N1-C2-N3	-18.19	120.20	129.30
22	BA	979	A	C2-N3-C4	18.19	119.70	110.60
1	AA	478	A	C2-N3-C4	18.19	119.69	110.60
1	AA	1413	A	N1-C2-N3	-18.19	120.20	129.30
22	BA	311	A	N1-C2-N3	-18.19	120.20	129.30
1	AA	704	A	N1-C2-N3	-18.19	120.20	129.30
1	AA	1016	A	N1-C2-N3	-18.19	120.21	129.30
1	AA	1437	A	N1-C2-N3	-18.19	120.21	129.30
22	BA	1610	A	N1-C2-N3	-18.19	120.20	129.30
1	AA	282	A	N1-C2-N3	-18.19	120.21	129.30
22	BA	382	A	N1-C2-N3	-18.19	120.21	129.30
22	BA	1641	A	C2-N3-C4	18.19	119.69	110.60
22	BA	556	A	N1-C6-N6	-18.19	107.69	118.60
22	BA	1080	A	C2-N3-C4	18.19	119.69	110.60
23	BB	53	A	N1-C2-N3	-18.19	120.21	129.30
1	AA	777	A	C2-N3-C4	18.18	119.69	110.60
22	BA	614	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	980	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	1614	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	2019	A	C2-N3-C4	18.18	119.69	110.60
22	BA	1284	A	C2-N3-C4	18.18	119.69	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	501	A	C2-N3-C4	18.18	119.69	110.60
22	BA	2268	A	N1-C2-N3	-18.18	120.21	129.30
1	AA	59	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	2211	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	2425	A	C2-N3-C4	18.18	119.69	110.60
1	AA	845	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	927	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	1700	A	C2-N3-C4	18.18	119.69	110.60
1	AA	205	A	C2-N3-C4	18.18	119.69	110.60
1	AA	205	A	N1-C6-N6	-18.18	107.69	118.60
1	AA	1287	A	C2-N3-C4	18.18	119.69	110.60
22	BA	346	A	C2-N3-C4	18.18	119.69	110.60
22	BA	443	A	C2-N3-C4	18.18	119.69	110.60
22	BA	2476	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	2837	A	N1-C2-N3	-18.18	120.21	129.30
55	B8	14	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	401	A	N1-C6-N6	-18.17	107.70	118.60
22	BA	1420	A	N1-C2-N3	-18.17	120.21	129.30
22	BA	1632	A	N1-C2-N3	-18.17	120.21	129.30
22	BA	1739	A	N1-C2-N3	-18.17	120.21	129.30
22	BA	2322	A	N1-C6-N6	-18.17	107.70	118.60
22	BA	2660	A	C2-N3-C4	18.17	119.69	110.60
1	AA	179	A	N1-C2-N3	-18.17	120.22	129.30
22	BA	2741	A	C2-N3-C4	18.17	119.69	110.60
22	BA	2821	A	N1-C2-N3	-18.17	120.22	129.30
1	AA	363	A	C2-N3-C4	18.17	119.68	110.60
1	AA	915	A	C2-N3-C4	18.17	119.68	110.60
1	AA	10	A	C2-N3-C4	18.17	119.68	110.60
1	AA	171	A	C2-N3-C4	18.17	119.68	110.60
22	BA	1953	A	N1-C6-N6	-18.17	107.70	118.60
1	AA	1368	A	N1-C6-N6	-18.17	107.70	118.60
22	BA	676	A	N1-C2-N3	-18.17	120.22	129.30
22	BA	1505	A	N1-C6-N6	-18.17	107.70	118.60
1	AA	1261	A	N1-C2-N3	-18.16	120.22	129.30
22	BA	1009	A	C2-N3-C4	18.16	119.68	110.60
22	BA	1098	A	C2-N3-C4	18.16	119.68	110.60
1	AA	964	A	N1-C6-N6	-18.16	107.70	118.60
22	BA	654	A	N1-C6-N6	-18.16	107.70	118.60
22	BA	1327	A	N1-C2-N3	-18.16	120.22	129.30
22	BA	2366	A	N1-C6-N6	-18.16	107.70	118.60
1	AA	975	A	N1-C2-N3	-18.16	120.22	129.30
22	BA	125	A	N1-C6-N6	-18.16	107.70	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	528	A	N1-C6-N6	-18.16	107.70	118.60
22	BA	1566	A	N1-C6-N6	-18.16	107.70	118.60
22	BA	1073	A	N1-C6-N6	-18.16	107.70	118.60
1	AA	155	A	C2-N3-C4	18.16	119.68	110.60
1	AA	535	A	N1-C6-N6	-18.16	107.71	118.60
1	AA	563	A	C2-N3-C4	18.16	119.68	110.60
1	AA	364	A	C2-N3-C4	18.15	119.68	110.60
1	AA	994	A	C2-N3-C4	18.15	119.68	110.60
1	AA	1430	A	C2-N3-C4	18.15	119.68	110.60
22	BA	1147	A	C2-N3-C4	18.15	119.68	110.60
22	BA	2287	A	C2-N3-C4	18.15	119.68	110.60
1	AA	749	A	N1-C6-N6	-18.15	107.71	118.60
22	BA	142	A	C2-N3-C4	18.15	119.67	110.60
22	BA	197	A	N1-C2-N3	-18.15	120.22	129.30
22	BA	1111	A	N1-C2-N3	-18.15	120.22	129.30
22	BA	1453	A	N1-C2-N3	-18.15	120.22	129.30
22	BA	1383	A	C2-N3-C4	18.15	119.67	110.60
1	AA	642	A	N1-C6-N6	-18.15	107.71	118.60
22	BA	391	A	C2-N3-C4	18.15	119.67	110.60
22	BA	1378	A	N1-C2-N3	-18.15	120.23	129.30
1	AA	1398	A	C2-N3-C4	18.14	119.67	110.60
22	BA	933	A	N1-C6-N6	-18.14	107.71	118.60
22	BA	2564	A	N1-C2-N3	-18.14	120.23	129.30
1	AA	1111	A	N1-C6-N6	-18.14	107.71	118.60
22	BA	218	A	C2-N3-C4	18.14	119.67	110.60
22	BA	689	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	1126	A	N1-C6-N6	-18.14	107.71	118.60
22	BA	1650	A	N1-C6-N6	-18.14	107.71	118.60
1	AA	1019	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	146	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	715	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	1336	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	2297	A	N1-C6-N6	-18.14	107.72	118.60
1	AA	1155	A	N1-C6-N6	-18.14	107.72	118.60
1	AA	415	A	N1-C6-N6	-18.14	107.72	118.60
1	AA	1171	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	348	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	2097	A	C2-N3-C4	18.14	119.67	110.60
23	BB	34	A	C2-N3-C4	18.14	119.67	110.60
22	BA	1366	A	C2-N3-C4	18.13	119.67	110.60
1	AA	65	A	N1-C6-N6	-18.13	107.72	118.60
22	BA	181	A	N1-C2-N3	-18.13	120.23	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2169	A	N1-C6-N6	-18.13	107.72	118.60
23	BB	94	A	N1-C6-N6	-18.13	107.72	118.60
1	AA	16	A	C2-N3-C4	18.13	119.67	110.60
22	BA	947	A	C2-N3-C4	18.13	119.67	110.60
22	BA	2094	A	C2-N3-C4	18.13	119.66	110.60
1	AA	968	A	N1-C6-N6	-18.13	107.72	118.60
22	BA	900	A	C2-N3-C4	18.13	119.66	110.60
22	BA	1095	A	N1-C6-N6	-18.13	107.72	118.60
22	BA	1246	A	C2-N3-C4	18.13	119.66	110.60
22	BA	2476	A	N1-C2-N3	-18.13	120.24	129.30
22	BA	1579	A	C2-N3-C4	18.12	119.66	110.60
1	AA	181	A	N1-C2-N3	-18.12	120.24	129.30
22	BA	142	A	N1-C6-N6	-18.12	107.73	118.60
22	BA	270	A	N1-C2-N3	-18.12	120.24	129.30
22	BA	344	A	C2-N3-C4	18.12	119.66	110.60
22	BA	1591	A	N1-C2-N3	-18.12	120.24	129.30
23	BB	53	A	C2-N3-C4	18.12	119.66	110.60
1	AA	728	A	N1-C6-N6	-18.12	107.73	118.60
22	BA	404	A	N1-C2-N3	-18.12	120.24	129.30
22	BA	1307	A	N1-C6-N6	-18.12	107.73	118.60
22	BA	1367	A	N1-C2-N3	-18.12	120.24	129.30
1	AA	250	A	N1-C6-N6	-18.12	107.73	118.60
1	AA	860	A	N1-C6-N6	-18.12	107.73	118.60
22	BA	1032	A	N1-C2-N3	-18.12	120.24	129.30
22	BA	2882	A	N1-C2-N3	-18.12	120.24	129.30
1	AA	1441	A	N1-C2-N3	-18.12	120.24	129.30
1	AA	432	A	N1-C6-N6	-18.11	107.73	118.60
22	BA	155	A	N1-C2-N3	-18.11	120.24	129.30
22	BA	503	A	N1-C6-N6	-18.11	107.73	118.60
22	BA	802	A	N1-C2-N3	-18.11	120.24	129.30
22	BA	1276	A	C2-N3-C4	18.11	119.66	110.60
22	BA	1383	A	N1-C2-N3	-18.11	120.24	129.30
22	BA	2800	A	N1-C2-N3	-18.11	120.24	129.30
22	BA	2813	A	C2-N3-C4	18.11	119.66	110.60
23	BB	119	A	C2-N3-C4	18.11	119.66	110.60
22	BA	981	A	C2-N3-C4	18.11	119.66	110.60
1	AA	696	A	C2-N3-C4	18.11	119.66	110.60
1	AA	814	A	C2-N3-C4	18.11	119.66	110.60
1	AA	907	A	C2-N3-C4	18.11	119.66	110.60
1	AA	1362	A	N1-C2-N3	-18.11	120.24	129.30
22	BA	204	A	N1-C2-N3	-18.11	120.25	129.30
22	BA	2883	A	N1-C2-N3	-18.11	120.25	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	330	A	N1-C2-N3	-18.11	120.25	129.30
55	B8	6	A	C2-N3-C4	18.11	119.65	110.60
1	AA	414	A	N1-C2-N3	-18.11	120.25	129.30
22	BA	402	A	C2-N3-C4	18.11	119.65	110.60
22	BA	1494	A	N1-C2-N3	-18.11	120.25	129.30
23	BB	50	A	N1-C2-N3	-18.11	120.25	129.30
55	B8	26	A	N1-C2-N3	-18.11	120.25	129.30
1	AA	1035	A	N1-C2-N3	-18.10	120.25	129.30
22	BA	1652	A	N1-C6-N6	-18.10	107.74	118.60
1	AA	179	A	C2-N3-C4	18.10	119.65	110.60
22	BA	38	A	C2-N3-C4	18.10	119.65	110.60
1	AA	1433	A	N1-C6-N6	-18.10	107.74	118.60
22	BA	2660	A	N1-C6-N6	-18.10	107.74	118.60
1	AA	535	A	N1-C2-N3	-18.10	120.25	129.30
22	BA	1373	A	C2-N3-C4	18.10	119.65	110.60
22	BA	1502	A	N1-C2-N3	-18.10	120.25	129.30
22	BA	1583	A	N1-C2-N3	-18.10	120.25	129.30
22	BA	1952	A	C2-N3-C4	18.10	119.65	110.60
1	AA	687	A	N1-C2-N3	-18.09	120.25	129.30
1	AA	694	A	N1-C6-N6	-18.09	107.74	118.60
22	BA	181	A	C2-N3-C4	18.09	119.65	110.60
23	BB	29	A	N1-C2-N3	-18.09	120.25	129.30
22	BA	272	A	C2-N3-C4	18.09	119.65	110.60
1	AA	236	A	N1-C2-N3	-18.09	120.25	129.30
22	BA	401	A	N1-C2-N3	-18.09	120.25	129.30
22	BA	631	A	C2-N3-C4	18.09	119.65	110.60
22	BA	1665	A	C2-N3-C4	18.09	119.65	110.60
22	BA	1786	A	C2-N3-C4	18.09	119.64	110.60
22	BA	2764	A	C2-N3-C4	18.09	119.64	110.60
1	AA	747	A	N1-C6-N6	-18.09	107.75	118.60
22	BA	1089	A	N1-C2-N3	-18.09	120.26	129.30
1	AA	583	A	C2-N3-C4	18.09	119.64	110.60
22	BA	1010	A	N1-C2-N3	-18.09	120.26	129.30
22	BA	1032	A	C2-N3-C4	18.09	119.64	110.60
22	BA	1080	A	N1-C6-N6	-18.09	107.75	118.60
22	BA	2158	A	N1-C6-N6	-18.09	107.75	118.60
1	AA	1092	A	N1-C2-N3	-18.08	120.26	129.30
1	AA	1246	A	N1-C2-N3	-18.08	120.26	129.30
1	AA	1042	A	N1-C2-N3	-18.08	120.26	129.30
1	AA	366	A	N1-C6-N6	-18.08	107.75	118.60
22	BA	1359	A	C2-N3-C4	18.08	119.64	110.60
1	AA	747	A	C2-N3-C4	18.08	119.64	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	371	A	C2-N3-C4	18.08	119.64	110.60
22	BA	1960	A	N1-C6-N6	-18.08	107.75	118.60
22	BA	2706	A	N1-C6-N6	-18.08	107.75	118.60
23	BB	78	A	N1-C2-N3	-18.08	120.26	129.30
1	AA	130	A	C2-N3-C4	18.07	119.64	110.60
1	AA	262	A	N1-C6-N6	-18.07	107.75	118.60
22	BA	1302	A	C2-N3-C4	18.07	119.64	110.60
22	BA	1328	A	C2-N3-C4	18.07	119.64	110.60
1	AA	747	A	N1-C2-N3	-18.07	120.26	129.30
22	BA	528	A	C2-N3-C4	18.07	119.64	110.60
22	BA	1384	A	N1-C2-N3	-18.07	120.27	129.30
22	BA	1503	A	N1-C6-N6	-18.07	107.76	118.60
22	BA	1757	A	N1-C6-N6	-18.07	107.76	118.60
1	AA	1022	A	N1-C2-N3	-18.07	120.27	129.30
1	AA	1396	A	C2-N3-C4	18.07	119.64	110.60
1	AA	704	A	C2-N3-C4	18.07	119.63	110.60
1	AA	1021	A	C2-N3-C4	18.07	119.63	110.60
1	AA	1152	A	N1-C6-N6	-18.07	107.76	118.60
1	AA	1219	A	C2-N3-C4	18.07	119.63	110.60
22	BA	1745	A	C2-N3-C4	18.07	119.64	110.60
22	BA	89	A	N1-C2-N3	-18.07	120.27	129.30
22	BA	654	A	C2-N3-C4	18.07	119.63	110.60
1	AA	1	A	N1-C2-N3	-18.07	120.27	129.30
1	AA	192	A	C2-N3-C4	18.07	119.63	110.60
1	AA	781	A	N1-C2-N3	-18.07	120.27	129.30
22	BA	2682	A	N1-C2-N3	-18.07	120.27	129.30
22	BA	91	A	N1-C2-N3	-18.06	120.27	129.30
22	BA	925	A	N1-C2-N3	-18.06	120.27	129.30
22	BA	1744	A	C2-N3-C4	18.06	119.63	110.60
1	AA	2	A	N1-C2-N3	-18.06	120.27	129.30
22	BA	532	A	N1-C2-N3	-18.06	120.27	129.30
22	BA	2675	A	C2-N3-C4	18.06	119.63	110.60
22	BA	1705	A	C2-N3-C4	18.06	119.63	110.60
22	BA	2497	A	C2-N3-C4	18.06	119.63	110.60
1	AA	559	A	N1-C6-N6	-18.06	107.77	118.60
22	BA	2675	A	N1-C2-N3	-18.06	120.27	129.30
1	AA	167	A	C2-N3-C4	18.06	119.63	110.60
22	BA	538	A	N1-C6-N6	-18.05	107.77	118.60
22	BA	2734	A	N1-C6-N6	-18.05	107.77	118.60
1	AA	1179	A	N1-C2-N3	-18.05	120.27	129.30
1	AA	1248	A	C2-N3-C4	18.05	119.63	110.60
1	AA	1447	A	C2-N3-C4	18.05	119.63	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1676	A	N1-C2-N3	-18.05	120.27	129.30
1	AA	749	A	C2-N3-C4	18.05	119.63	110.60
1	AA	1254	A	N1-C6-N6	-18.05	107.77	118.60
55	B8	41	A	N1-C2-N3	-18.05	120.27	129.30
1	AA	1349	A	N1-C2-N3	-18.05	120.28	129.30
22	BA	2518	A	N1-C2-N3	-18.05	120.28	129.30
22	BA	1247	A	C2-N3-C4	18.05	119.62	110.60
1	AA	609	A	C2-N3-C4	18.05	119.62	110.60
22	BA	909	A	C2-N3-C4	18.05	119.62	110.60
22	BA	1572	A	C2-N3-C4	18.05	119.62	110.60
1	AA	878	A	N1-C2-N3	-18.04	120.28	129.30
1	AA	602	A	C2-N3-C4	18.04	119.62	110.60
22	BA	1169	A	N1-C6-N6	-18.04	107.78	118.60
23	BB	119	A	N1-C2-N3	-18.04	120.28	129.30
1	AA	1318	A	C2-N3-C4	18.04	119.62	110.60
22	BA	1654	A	C2-N3-C4	18.04	119.62	110.60
22	BA	1803	A	N1-C6-N6	-18.04	107.78	118.60
1	AA	303	A	C2-N3-C4	18.04	119.62	110.60
1	AA	1256	A	N1-C2-N3	-18.04	120.28	129.30
22	BA	454	A	N1-C2-N3	-18.04	120.28	129.30
22	BA	1690	A	N1-C6-N6	-18.04	107.78	118.60
22	BA	2602	A	N1-C2-N3	-18.04	120.28	129.30
22	BA	1050	A	C2-N3-C4	18.04	119.62	110.60
22	BA	2298	A	N1-C2-N3	-18.03	120.28	129.30
22	BA	2635	A	N1-C2-N3	-18.03	120.28	129.30
22	BA	2665	A	N1-C6-N6	-18.03	107.78	118.60
23	BB	52	A	N1-C2-N3	-18.03	120.28	129.30
22	BA	1230	A	N1-C2-N3	-18.03	120.28	129.30
22	BA	2183	A	N1-C2-N3	-18.03	120.28	129.30
22	BA	1020	A	C2-N3-C4	18.03	119.62	110.60
22	BA	1509	A	N1-C6-N6	-18.03	107.78	118.60
1	AA	495	A	N1-C2-N3	-18.03	120.28	129.30
1	AA	1318	A	N1-C2-N3	-18.03	120.28	129.30
1	AA	1346	A	N1-C2-N3	-18.03	120.29	129.30
22	BA	721	A	C2-N3-C4	18.03	119.61	110.60
22	BA	2634	A	N1-C2-N3	-18.03	120.29	129.30
22	BA	2800	A	N1-C6-N6	-18.03	107.78	118.60
22	BA	2014	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	181	A	N1-C6-N6	-18.02	107.79	118.60
22	BA	666	A	C2-N3-C4	18.02	119.61	110.60
1	AA	149	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	896	A	N1-C2-N3	-18.02	120.29	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1040	A	N1-C6-N6	-18.02	107.79	118.60
1	AA	718	A	C2-N3-C4	18.02	119.61	110.60
22	BA	155	A	C2-N3-C4	18.02	119.61	110.60
22	BA	2352	A	C2-N3-C4	18.02	119.61	110.60
1	AA	315	A	N1-C2-N3	-18.02	120.29	129.30
1	AA	759	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	5	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	538	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	1912	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	2119	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	2530	A	N1-C6-N6	-18.02	107.79	118.60
1	AA	101	A	N1-C6-N6	-18.02	107.79	118.60
1	AA	523	A	N1-C6-N6	-18.02	107.79	118.60
22	BA	56	A	C2-N3-C4	18.02	119.61	110.60
22	BA	586	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	1669	A	C2-N3-C4	18.02	119.61	110.60
22	BA	1713	A	N1-C6-N6	-18.02	107.79	118.60
22	BA	1981	A	N1-C2-N3	-18.02	120.29	129.30
1	AA	78	A	N1-C2-N3	-18.01	120.29	129.30
1	AA	189	A	N1-C2-N3	-18.01	120.29	129.30
22	BA	371	A	N1-C2-N3	-18.01	120.29	129.30
22	BA	2095	A	C2-N3-C4	18.01	119.61	110.60
22	BA	176	A	N1-C2-N3	-18.01	120.29	129.30
22	BA	2366	A	N1-C2-N3	-18.01	120.29	129.30
22	BA	226	A	N1-C6-N6	-18.01	107.79	118.60
1	AA	344	A	C2-N3-C4	18.01	119.60	110.60
1	AA	414	A	C2-N3-C4	18.01	119.61	110.60
1	AA	1288	A	N1-C2-N3	-18.01	120.30	129.30
22	BA	1328	A	N1-C6-N6	-18.01	107.80	118.60
22	BA	1470	A	N1-C6-N6	-18.01	107.80	118.60
22	BA	1805	A	N1-C2-N3	-18.01	120.30	129.30
1	AA	161	A	C2-N3-C4	18.00	119.60	110.60
1	AA	968	A	N1-C2-N3	-18.00	120.30	129.30
1	AA	1513	A	N1-C2-N3	-18.00	120.30	129.30
22	BA	216	A	C2-N3-C4	18.00	119.60	110.60
22	BA	330	A	N1-C6-N6	-18.00	107.80	118.60
22	BA	676	A	C2-N3-C4	18.00	119.60	110.60
22	BA	1960	A	N1-C2-N3	-18.00	120.30	129.30
23	BB	109	A	N1-C2-N3	-18.00	120.30	129.30
1	AA	149	A	C2-N3-C4	18.00	119.60	110.60
22	BA	483	A	C2-N3-C4	18.00	119.60	110.60
22	BA	575	A	N1-C2-N3	-18.00	120.30	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1088	A	C2-N3-C4	18.00	119.60	110.60
22	BA	2883	A	C2-N3-C4	18.00	119.60	110.60
1	AA	192	A	N1-C6-N6	-18.00	107.80	118.60
1	AA	1248	A	N1-C2-N3	-18.00	120.30	129.30
22	BA	574	A	N1-C2-N3	-18.00	120.30	129.30
22	BA	918	A	C2-N3-C4	18.00	119.60	110.60
1	AA	1398	A	N1-C2-N3	-18.00	120.30	129.30
22	BA	1307	A	C2-N3-C4	18.00	119.60	110.60
1	AA	109	A	N1-C6-N6	-18.00	107.80	118.60
1	AA	1117	A	N1-C6-N6	-18.00	107.80	118.60
23	BB	57	A	C2-N3-C4	18.00	119.60	110.60
1	AA	695	A	N1-C6-N6	-18.00	107.80	118.60
1	AA	1285	A	C2-N3-C4	18.00	119.60	110.60
1	AA	1332	A	N1-C2-N3	-18.00	120.30	129.30
22	BA	2851	A	N1-C2-N3	-18.00	120.30	129.30
22	BA	2899	A	C2-N3-C4	18.00	119.60	110.60
23	BB	108	A	N1-C6-N6	-18.00	107.80	118.60
1	AA	994	A	N1-C6-N6	-17.99	107.80	118.60
22	BA	845	A	N1-C2-N3	-17.99	120.30	129.30
1	AA	1157	A	N1-C6-N6	-17.99	107.80	118.60
1	AA	1254	A	C2-N3-C4	17.99	119.59	110.60
1	AA	780	A	C2-N3-C4	17.99	119.59	110.60
22	BA	1453	A	C2-N3-C4	17.99	119.59	110.60
22	BA	1819	A	N1-C2-N3	-17.99	120.31	129.30
22	BA	1854	A	C2-N3-C4	17.99	119.59	110.60
1	AA	1257	A	C2-N3-C4	17.99	119.59	110.60
22	BA	2900	A	C2-N3-C4	17.99	119.59	110.60
1	AA	71	A	N1-C2-N3	-17.98	120.31	129.30
22	BA	2711	A	N1-C2-N3	-17.98	120.31	129.30
22	BA	2776	A	C2-N3-C4	17.98	119.59	110.60
1	AA	487	A	C2-N3-C4	17.98	119.59	110.60
22	BA	1175	A	N1-C2-N3	-17.98	120.31	129.30
22	BA	1304	A	N1-C2-N3	-17.98	120.31	129.30
22	BA	1508	A	N1-C2-N3	-17.98	120.31	129.30
23	BB	15	A	C2-N3-C4	17.98	119.59	110.60
1	AA	743	A	C2-N3-C4	17.98	119.59	110.60
1	AA	1225	A	N1-C2-N3	-17.98	120.31	129.30
22	BA	920	A	N1-C2-N3	-17.98	120.31	129.30
22	BA	2541	A	N1-C2-N3	-17.98	120.31	129.30
22	BA	428	A	N1-C6-N6	-17.97	107.81	118.60
1	AA	907	A	N1-C2-N3	-17.97	120.31	129.30
1	AA	1082	A	N1-C6-N6	-17.97	107.82	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1609	A	C2-N3-C4	17.97	119.59	110.60
1	AA	478	A	N1-C2-N3	-17.97	120.31	129.30
22	BA	156	A	C2-N3-C4	17.97	119.58	110.60
1	AA	873	A	N1-C2-N3	-17.97	120.31	129.30
1	AA	1067	A	C2-N3-C4	17.97	119.58	110.60
22	BA	345	A	C2-N3-C4	17.97	119.58	110.60
22	BA	616	A	C2-N3-C4	17.97	119.58	110.60
22	BA	2058	A	N1-C2-N3	-17.97	120.31	129.30
22	BA	2336	A	N1-C2-N3	-17.97	120.31	129.30
1	AA	1257	A	N1-C2-N3	-17.97	120.32	129.30
22	BA	613	A	N1-C6-N6	-17.97	107.82	118.60
1	AA	279	A	N1-C6-N6	-17.97	107.82	118.60
1	AA	1019	A	C2-N3-C4	17.97	119.58	110.60
1	AA	1167	A	N1-C2-N3	-17.96	120.32	129.30
1	AA	609	A	N1-C2-N3	-17.96	120.32	129.30
1	AA	872	A	N1-C2-N3	-17.96	120.32	129.30
1	AA	3	A	N1-C2-N3	-17.96	120.32	129.30
1	AA	523	A	C2-N3-C4	17.96	119.58	110.60
1	AA	864	A	C2-N3-C4	17.96	119.58	110.60
22	BA	1871	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	2227	A	N1-C6-N6	-17.96	107.82	118.60
1	AA	996	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	556	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	1039	A	N1-C2-N3	-17.96	120.32	129.30
55	B8	14	A	C2-N3-C4	17.96	119.58	110.60
22	BA	309	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	2810	A	N1-C2-N3	-17.96	120.32	129.30
1	AA	1191	A	N1-C2-N3	-17.95	120.32	129.30
1	AA	1213	A	C2-N3-C4	17.95	119.58	110.60
22	BA	574	A	C2-N3-C4	17.95	119.58	110.60
22	BA	1347	A	N1-C2-N3	-17.95	120.32	129.30
22	BA	2665	A	N1-C2-N3	-17.95	120.32	129.30
1	AA	119	A	N1-C2-N3	-17.95	120.32	129.30
22	BA	1189	A	N1-C2-N3	-17.95	120.32	129.30
22	BA	1274	A	N1-C2-N3	-17.95	120.32	129.30
22	BA	1495	A	N1-C2-N3	-17.95	120.32	129.30
22	BA	2288	A	C2-N3-C4	17.95	119.58	110.60
22	BA	2711	A	N1-C6-N6	-17.95	107.83	118.60
1	AA	19	A	C2-N3-C4	17.95	119.57	110.60
1	AA	629	A	C2-N3-C4	17.95	119.57	110.60
22	BA	227	A	N1-C2-N3	-17.95	120.33	129.30
22	BA	749	A	C2-N3-C4	17.95	119.57	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1821	A	N1-C2-N3	-17.95	120.33	129.30
22	BA	2750	A	C2-N3-C4	17.95	119.57	110.60
1	AA	908	A	N1-C2-N3	-17.95	120.33	129.30
22	BA	1111	A	C2-N3-C4	17.95	119.57	110.60
22	BA	1847	A	N1-C2-N3	-17.95	120.33	129.30
22	BA	1969	A	N1-C6-N6	-17.95	107.83	118.60
1	AA	1374	A	C2-N3-C4	17.94	119.57	110.60
22	BA	2388	A	C2-N3-C4	17.94	119.57	110.60
1	AA	364	A	N1-C2-N3	-17.94	120.33	129.30
1	AA	892	A	N1-C2-N3	-17.94	120.33	129.30
22	BA	144	A	C2-N3-C4	17.94	119.57	110.60
22	BA	320	A	C2-N3-C4	17.94	119.57	110.60
22	BA	402	A	N1-C2-N3	-17.94	120.33	129.30
1	AA	1275	A	N1-C2-N3	-17.94	120.33	129.30
22	BA	1744	A	N1-C2-N3	-17.94	120.33	129.30
22	BA	1966	A	N1-C6-N6	-17.94	107.84	118.60
22	BA	2191	A	N1-C2-N3	-17.94	120.33	129.30
22	BA	2369	A	C2-N3-C4	17.94	119.57	110.60
22	BA	2560	A	N1-C2-N3	-17.94	120.33	129.30
1	AA	129	A	N1-C2-N3	-17.94	120.33	129.30
1	AA	243	A	C2-N3-C4	17.94	119.57	110.60
22	BA	2856	A	N1-C2-N3	-17.94	120.33	129.30
22	BA	2868	A	N1-C2-N3	-17.94	120.33	129.30
22	BA	345	A	N1-C2-N3	-17.93	120.33	129.30
22	BA	1596	A	N1-C2-N3	-17.93	120.33	129.30
22	BA	1787	A	N1-C6-N6	-17.93	107.84	118.60
23	BB	94	A	N1-C2-N3	-17.93	120.33	129.30
1	AA	78	A	C2-N3-C4	17.93	119.57	110.60
22	BA	2758	A	N1-C2-N3	-17.93	120.33	129.30
22	BA	1046	A	N1-C2-N3	-17.93	120.33	129.30
22	BA	2205	A	N1-C6-N6	-17.93	107.84	118.60
22	BA	925	A	N1-C6-N6	-17.93	107.84	118.60
1	AA	16	A	N1-C2-N3	-17.93	120.34	129.30
1	AA	831	A	N1-C6-N6	-17.93	107.84	118.60
1	AA	1014	A	C2-N3-C4	17.93	119.56	110.60
1	AA	1176	A	C2-N3-C4	17.93	119.56	110.60
1	AA	1229	A	N1-C2-N3	-17.93	120.34	129.30
22	BA	1504	A	N1-C2-N3	-17.93	120.34	129.30
23	BB	99	A	N1-C2-N3	-17.93	120.34	129.30
1	AA	131	A	N1-C2-N3	-17.93	120.34	129.30
1	AA	1196	A	N1-C6-N6	-17.93	107.84	118.60
1	AA	607	A	C2-N3-C4	17.92	119.56	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	900	A	C2-N3-C4	17.92	119.56	110.60
22	BA	344	A	N1-C6-N6	-17.92	107.85	118.60
22	BA	526	A	C2-N3-C4	17.92	119.56	110.60
1	AA	441	A	C2-N3-C4	17.92	119.56	110.60
1	AA	456	A	C2-N3-C4	17.92	119.56	110.60
22	BA	320	A	N1-C2-N3	-17.92	120.34	129.30
22	BA	501	A	N1-C2-N3	-17.92	120.34	129.30
22	BA	1998	A	N1-C2-N3	-17.92	120.34	129.30
22	BA	2268	A	C2-N3-C4	17.92	119.56	110.60
22	BA	2899	A	N1-C2-N3	-17.92	120.34	129.30
1	AA	199	A	C2-N3-C4	17.92	119.56	110.60
22	BA	2412	A	N1-C6-N6	-17.92	107.85	118.60
1	AA	155	A	N1-C2-N3	-17.91	120.34	129.30
1	AA	160	A	C2-N3-C4	17.91	119.56	110.60
1	AA	415	A	C2-N3-C4	17.91	119.56	110.60
22	BA	344	A	N1-C2-N3	-17.91	120.34	129.30
22	BA	422	A	N1-C6-N6	-17.91	107.85	118.60
22	BA	1287	A	N1-C6-N6	-17.91	107.85	118.60
22	BA	1434	A	C2-N3-C4	17.91	119.56	110.60
22	BA	2171	A	C2-N3-C4	17.91	119.56	110.60
1	AA	161	A	N1-C2-N3	-17.91	120.34	129.30
22	BA	52	A	C2-N3-C4	17.91	119.56	110.60
1	AA	1275	A	C2-N3-C4	17.91	119.55	110.60
22	BA	1713	A	C2-N3-C4	17.91	119.55	110.60
22	BA	2381	A	N1-C2-N3	-17.91	120.35	129.30
1	AA	1151	A	C2-N3-C4	17.91	119.55	110.60
22	BA	918	A	N1-C2-N3	-17.91	120.35	129.30
22	BA	2346	A	C2-N3-C4	17.91	119.55	110.60
22	BA	2809	A	C2-N3-C4	17.91	119.55	110.60
22	BA	149	A	C2-N3-C4	17.90	119.55	110.60
22	BA	1591	A	C2-N3-C4	17.90	119.55	110.60
22	BA	1900	A	N1-C2-N3	-17.90	120.35	129.30
22	BA	2792	A	N1-C2-N3	-17.90	120.35	129.30
1	AA	80	A	N1-C2-N3	-17.90	120.35	129.30
1	AA	1394	A	C2-N3-C4	17.90	119.55	110.60
22	BA	1676	A	N1-C6-N6	-17.90	107.86	118.60
22	BA	2070	A	N1-C6-N6	-17.90	107.86	118.60
22	BA	666	A	N1-C2-N3	-17.90	120.35	129.30
22	BA	1532	A	N1-C2-N3	-17.90	120.35	129.30
22	BA	2134	A	N1-C2-N3	-17.90	120.35	129.30
1	AA	77	A	C2-N3-C4	17.90	119.55	110.60
1	AA	432	A	C2-N3-C4	17.90	119.55	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	699	A	N1-C2-N3	-17.90	120.35	129.30
22	BA	1021	A	C2-N3-C4	17.90	119.55	110.60
22	BA	1147	A	N1-C6-N6	-17.90	107.86	118.60
1	AA	706	A	C2-N3-C4	17.90	119.55	110.60
1	AA	205	A	N1-C2-N3	-17.90	120.35	129.30
1	AA	432	A	N1-C2-N3	-17.90	120.35	129.30
1	AA	451	A	N1-C6-N6	-17.90	107.86	118.60
1	AA	465	A	C2-N3-C4	17.90	119.55	110.60
1	AA	900	A	N1-C2-N3	-17.90	120.35	129.30
22	BA	2311	A	N1-C2-N3	-17.90	120.35	129.30
22	BA	2886	A	N1-C2-N3	-17.90	120.35	129.30
55	B8	21	A	C2-N3-C4	17.90	119.55	110.60
22	BA	2170	A	C2-N3-C4	17.89	119.55	110.60
23	BB	15	A	N1-C2-N3	-17.89	120.35	129.30
1	AA	600	A	N1-C6-N6	-17.89	107.86	118.60
1	AA	1256	A	C2-N3-C4	17.89	119.55	110.60
22	BA	2335	A	C2-N3-C4	17.89	119.55	110.60
1	AA	238	A	N1-C2-N3	-17.89	120.35	129.30
1	AA	784	A	C2-N3-C4	17.89	119.55	110.60
22	BA	2173	A	N1-C2-N3	-17.89	120.35	129.30
22	BA	1095	A	C2-N3-C4	17.89	119.55	110.60
22	BA	1342	A	C2-N3-C4	17.89	119.55	110.60
22	BA	2077	A	C2-N3-C4	17.89	119.55	110.60
22	BA	2314	A	N1-C2-N3	-17.89	120.36	129.30
22	BA	2654	A	N1-C6-N6	-17.89	107.86	118.60
1	AA	1081	A	N1-C6-N6	-17.89	107.87	118.60
22	BA	547	A	N1-C2-N3	-17.89	120.36	129.30
22	BA	896	A	N1-C6-N6	-17.89	107.87	118.60
22	BA	1090	A	C2-N3-C4	17.89	119.54	110.60
1	AA	1239	A	C2-N3-C4	17.89	119.54	110.60
22	BA	300	A	N1-C6-N6	-17.89	107.87	118.60
23	BB	34	A	N1-C2-N3	-17.89	120.36	129.30
22	BA	1637	A	C2-N3-C4	17.88	119.54	110.60
1	AA	974	A	C2-N3-C4	17.88	119.54	110.60
22	BA	632	A	N1-C2-N3	-17.88	120.36	129.30
22	BA	1096	A	N1-C6-N6	-17.88	107.87	118.60
22	BA	2176	A	N1-C6-N6	-17.88	107.87	118.60
1	AA	167	A	N1-C2-N3	-17.88	120.36	129.30
1	AA	223	A	C2-N3-C4	17.88	119.54	110.60
1	AA	461	A	N1-C6-N6	-17.88	107.87	118.60
22	BA	1151	A	N1-C2-N3	-17.88	120.36	129.30
22	BA	1336	A	N1-C6-N6	-17.88	107.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1347	A	C2-N3-C4	17.88	119.54	110.60
1	AA	44	A	N1-C2-N3	-17.88	120.36	129.30
1	AA	1413	A	C2-N3-C4	17.88	119.54	110.60
22	BA	2328	A	N1-C2-N3	-17.88	120.36	129.30
1	AA	831	A	C2-N3-C4	17.88	119.54	110.60
22	BA	1050	A	N1-C2-N3	-17.88	120.36	129.30
22	BA	1505	A	C2-N3-C4	17.88	119.54	110.60
22	BA	2184	A	C2-N3-C4	17.88	119.54	110.60
22	BA	2227	A	C2-N3-C4	17.88	119.54	110.60
1	AA	374	A	N1-C2-N3	-17.87	120.36	129.30
22	BA	173	A	N1-C2-N3	-17.87	120.36	129.30
22	BA	1698	A	N1-C2-N3	-17.87	120.36	129.30
22	BA	1927	A	N1-C2-N3	-17.87	120.36	129.30
22	BA	1969	A	C2-N3-C4	17.87	119.54	110.60
22	BA	2309	A	N1-C2-N3	-17.87	120.36	129.30
22	BA	933	A	N1-C2-N3	-17.87	120.36	129.30
22	BA	2037	A	C2-N3-C4	17.87	119.54	110.60
22	BA	609	A	N1-C2-N3	-17.87	120.36	129.30
22	BA	2435	A	C2-N3-C4	17.87	119.53	110.60
22	BA	382	A	N1-C6-N6	-17.87	107.88	118.60
22	BA	592	A	N1-C2-N3	-17.87	120.36	129.30
22	BA	1987	A	N1-C6-N6	-17.87	107.88	118.60
1	AA	1036	A	N1-C2-N3	-17.87	120.37	129.30
1	AA	1197	A	C2-N3-C4	17.87	119.53	110.60
1	AA	1534	A	N1-C6-N6	-17.87	107.88	118.60
22	BA	167	A	C2-N3-C4	17.87	119.53	110.60
22	BA	439	A	N1-C2-N3	-17.87	120.37	129.30
22	BA	941	A	N1-C2-N3	-17.87	120.37	129.30
22	BA	2009	A	C2-N3-C4	17.87	119.53	110.60
1	AA	228	A	N1-C2-N3	-17.87	120.37	129.30
1	AA	468	A	N1-C6-N6	-17.87	107.88	118.60
1	AA	794	A	N1-C6-N6	-17.86	107.88	118.60
22	BA	1347	A	N1-C6-N6	-17.86	107.88	118.60
1	AA	1117	A	C2-N3-C4	17.86	119.53	110.60
22	BA	1676	A	C2-N3-C4	17.86	119.53	110.60
1	AA	130	A	N1-C6-N6	-17.86	107.88	118.60
1	AA	1111	A	C2-N3-C4	17.86	119.53	110.60
22	BA	191	A	N1-C2-N3	-17.86	120.37	129.30
22	BA	643	A	C2-N3-C4	17.86	119.53	110.60
22	BA	718	A	N1-C6-N6	-17.86	107.88	118.60
1	AA	694	A	N1-C2-N3	-17.86	120.37	129.30
1	AA	695	A	C2-N3-C4	17.86	119.53	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	233	A	N1-C2-N3	-17.86	120.37	129.30
22	BA	792	A	N1-C2-N3	-17.86	120.37	129.30
1	AA	908	A	C2-N3-C4	17.86	119.53	110.60
1	AA	968	A	C2-N3-C4	17.86	119.53	110.60
1	AA	1410	A	N1-C2-N3	-17.86	120.37	129.30
22	BA	996	A	N1-C2-N3	-17.86	120.37	129.30
22	BA	1096	A	C2-N3-C4	17.86	119.53	110.60
22	BA	1858	A	N1-C2-N3	-17.86	120.37	129.30
22	BA	2147	A	N1-C2-N3	-17.86	120.37	129.30
1	AA	1251	A	N1-C2-N3	-17.85	120.37	129.30
1	AA	1306	A	C2-N3-C4	17.85	119.53	110.60
22	BA	2381	A	C2-N3-C4	17.85	119.53	110.60
22	BA	2433	A	C2-N3-C4	17.85	119.53	110.60
22	BA	2753	A	N1-C2-N3	-17.85	120.37	129.30
1	AA	408	A	N1-C2-N3	-17.85	120.37	129.30
1	AA	975	A	C2-N3-C4	17.85	119.53	110.60
22	BA	936	A	N1-C2-N3	-17.85	120.38	129.30
22	BA	1027	A	C2-N3-C4	17.85	119.53	110.60
22	BA	1749	A	N1-C6-N6	-17.85	107.89	118.60
1	AA	1102	A	C2-N3-C4	17.85	119.52	110.60
22	BA	547	A	C2-N3-C4	17.85	119.52	110.60
22	BA	2765	A	N1-C2-N3	-17.85	120.38	129.30
1	AA	250	A	N1-C2-N3	-17.85	120.38	129.30
22	BA	2799	A	N1-C2-N3	-17.85	120.38	129.30
1	AA	223	A	N1-C6-N6	-17.84	107.89	118.60
22	BA	1431	A	C2-N3-C4	17.84	119.52	110.60
22	BA	2335	A	N1-C6-N6	-17.84	107.89	118.60
1	AA	1280	A	C2-N3-C4	17.84	119.52	110.60
22	BA	89	A	C2-N3-C4	17.84	119.52	110.60
1	AA	1005	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	1509	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	2170	A	N1-C6-N6	-17.84	107.89	118.60
22	BA	2328	A	N1-C6-N6	-17.84	107.89	118.60
1	AA	560	A	N1-C6-N6	-17.84	107.90	118.60
22	BA	64	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	1502	A	C2-N3-C4	17.84	119.52	110.60
1	AA	456	A	N1-C6-N6	-17.84	107.90	118.60
1	AA	1155	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	1705	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	1937	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	2225	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	38	A	N1-C2-N3	-17.83	120.38	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2014	A	C2-N3-C4	17.83	119.52	110.60
22	BA	483	A	N1-C2-N3	-17.83	120.38	129.30
22	BA	1039	A	C2-N3-C4	17.83	119.52	110.60
22	BA	1169	A	C2-N3-C4	17.83	119.52	110.60
1	AA	1093	A	N1-C6-N6	-17.83	107.90	118.60
22	BA	131	A	C2-N3-C4	17.83	119.52	110.60
22	BA	161	A	N1-C2-N3	-17.83	120.39	129.30
22	BA	1089	A	C2-N3-C4	17.83	119.51	110.60
22	BA	1689	A	C2-N3-C4	17.83	119.51	110.60
22	BA	2147	A	C2-N3-C4	17.83	119.51	110.60
22	BA	2170	A	N1-C2-N3	-17.83	120.39	129.30
1	AA	50	A	N1-C2-N3	-17.83	120.39	129.30
22	BA	2135	A	N1-C6-N6	-17.83	107.91	118.60
1	AA	71	A	N1-C6-N6	-17.82	107.91	118.60
1	AA	482	A	N1-C2-N3	-17.82	120.39	129.30
1	AA	766	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	101	A	C2-N3-C4	17.82	119.51	110.60
22	BA	2101	A	C2-N3-C4	17.82	119.51	110.60
22	BA	2278	A	N1-C6-N6	-17.82	107.91	118.60
23	BB	57	A	N1-C6-N6	-17.82	107.91	118.60
1	AA	81	A	N1-C2-N3	-17.82	120.39	129.30
1	AA	1465	A	C2-N3-C4	17.82	119.51	110.60
1	AA	80	A	C2-N3-C4	17.82	119.51	110.60
22	BA	1916	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	2071	A	N1-C6-N6	-17.82	107.91	118.60
1	AA	321	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	1073	A	C2-N3-C4	17.82	119.51	110.60
22	BA	2211	A	C2-N3-C4	17.82	119.51	110.60
22	BA	722	A	C2-N3-C4	17.82	119.51	110.60
22	BA	794	A	N1-C6-N6	-17.81	107.91	118.60
1	AA	28	A	C2-N3-C4	17.81	119.51	110.60
1	AA	196	A	N1-C2-N3	-17.81	120.39	129.30
22	BA	2273	A	N1-C6-N6	-17.81	107.91	118.60
1	AA	553	A	N1-C2-N3	-17.81	120.40	129.30
1	AA	937	A	C2-N3-C4	17.81	119.50	110.60
1	AA	1350	A	N1-C6-N6	-17.81	107.92	118.60
22	BA	282	A	N1-C2-N3	-17.81	120.39	129.30
22	BA	693	A	N1-C6-N6	-17.81	107.91	118.60
22	BA	2369	A	N1-C2-N3	-17.81	120.39	129.30
1	AA	382	A	N1-C6-N6	-17.81	107.92	118.60
1	AA	780	A	N1-C6-N6	-17.81	107.92	118.60
1	AA	974	A	N1-C6-N6	-17.81	107.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1396	A	N1-C2-N3	-17.81	120.40	129.30
55	B8	76	A	N1-C6-N6	-17.81	107.92	118.60
1	AA	270	A	C2-N3-C4	17.80	119.50	110.60
22	BA	1603	A	N1-C6-N6	-17.80	107.92	118.60
23	BB	45	A	C2-N3-C4	17.80	119.50	110.60
1	AA	7	A	C2-N3-C4	17.80	119.50	110.60
1	AA	451	A	N1-C2-N3	-17.80	120.40	129.30
1	AA	814	A	N1-C2-N3	-17.80	120.40	129.30
22	BA	28	A	C2-N3-C4	17.80	119.50	110.60
22	BA	1580	A	C2-N3-C4	17.80	119.50	110.60
22	BA	2482	A	C2-N3-C4	17.80	119.50	110.60
1	AA	1236	A	C2-N3-C4	17.80	119.50	110.60
1	AA	780	A	N1-C2-N3	-17.80	120.40	129.30
1	AA	1431	A	N1-C2-N3	-17.80	120.40	129.30
22	BA	1549	A	N1-C2-N3	-17.80	120.40	129.30
1	AA	44	A	C2-N3-C4	17.80	119.50	110.60
1	AA	996	A	C2-N3-C4	17.80	119.50	110.60
1	AA	10	A	N1-C2-N3	-17.80	120.40	129.30
22	BA	721	A	N1-C2-N3	-17.80	120.40	129.30
22	BA	1127	A	C2-N3-C4	17.80	119.50	110.60
1	AA	321	A	C2-N3-C4	17.79	119.50	110.60
1	AA	451	A	C2-N3-C4	17.79	119.50	110.60
22	BA	2748	A	C2-N3-C4	17.79	119.50	110.60
22	BA	643	A	N1-C6-N6	-17.79	107.93	118.60
1	AA	65	A	N1-C2-N3	-17.79	120.41	129.30
1	AA	468	A	C2-N3-C4	17.79	119.50	110.60
22	BA	56	A	N1-C6-N6	-17.79	107.93	118.60
1	AA	143	A	C2-N3-C4	17.79	119.49	110.60
22	BA	460	A	N1-C6-N6	-17.79	107.93	118.60
1	AA	630	A	N1-C2-N3	-17.78	120.41	129.30
1	AA	1146	A	N1-C2-N3	-17.78	120.41	129.30
1	AA	621	A	N1-C2-N3	-17.78	120.41	129.30
22	BA	2183	A	C2-N3-C4	17.78	119.49	110.60
1	AA	595	A	N1-C2-N3	-17.78	120.41	129.30
1	AA	949	A	N1-C2-N3	-17.78	120.41	129.30
22	BA	734	A	C2-N3-C4	17.78	119.49	110.60
22	BA	454	A	C2-N3-C4	17.78	119.49	110.60
1	AA	1360	A	C2-N3-C4	17.78	119.49	110.60
22	BA	503	A	C2-N3-C4	17.78	119.49	110.60
22	BA	1901	A	N1-C2-N3	-17.78	120.41	129.30
23	BB	52	A	N1-C6-N6	-17.78	107.93	118.60
1	AA	129	A	C2-N3-C4	17.77	119.49	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1428	A	N1-C2-N3	-17.77	120.41	129.30
22	BA	677	A	N1-C2-N3	-17.77	120.41	129.30
22	BA	1810	A	C2-N3-C4	17.77	119.49	110.60
22	BA	2434	A	C2-N3-C4	17.77	119.49	110.60
1	AA	595	A	C2-N3-C4	17.77	119.49	110.60
22	BA	2654	A	N1-C2-N3	-17.77	120.41	129.30
1	AA	1145	A	C2-N3-C4	17.77	119.48	110.60
22	BA	14	A	N1-C6-N6	-17.77	107.94	118.60
22	BA	354	A	N1-C6-N6	-17.77	107.94	118.60
1	AA	3	A	C2-N3-C4	17.77	119.48	110.60
1	AA	1434	A	N1-C2-N3	-17.77	120.42	129.30
22	BA	53	A	C2-N3-C4	17.77	119.48	110.60
22	BA	844	A	C2-N3-C4	17.77	119.48	110.60
22	BA	996	A	C2-N3-C4	17.77	119.48	110.60
1	AA	914	A	C2-N3-C4	17.77	119.48	110.60
22	BA	833	A	C2-N3-C4	17.77	119.48	110.60
22	BA	1098	A	N1-C2-N3	-17.77	120.42	129.30
22	BA	1142	A	N1-C2-N3	-17.77	120.42	129.30
1	AA	1227	A	N1-C6-N6	-17.76	107.94	118.60
22	BA	5	A	N1-C6-N6	-17.76	107.94	118.60
22	BA	203	A	N1-C2-N3	-17.76	120.42	129.30
22	BA	428	A	N1-C2-N3	-17.76	120.42	129.30
22	BA	676	A	N1-C6-N6	-17.76	107.94	118.60
22	BA	1103	A	C2-N3-C4	17.76	119.48	110.60
22	BA	2119	A	C2-N3-C4	17.76	119.48	110.60
22	BA	2705	A	N1-C2-N3	-17.76	120.42	129.30
1	AA	865	A	C2-N3-C4	17.76	119.48	110.60
1	AA	1000	A	C2-N3-C4	17.76	119.48	110.60
22	BA	2750	A	N1-C6-N6	-17.76	107.94	118.60
1	AA	509	A	N1-C2-N3	-17.76	120.42	129.30
1	AA	923	A	C2-N3-C4	17.76	119.48	110.60
1	AA	1167	A	N1-C6-N6	-17.76	107.94	118.60
22	BA	590	A	C2-N3-C4	17.76	119.48	110.60
22	BA	340	A	C2-N3-C4	17.75	119.48	110.60
22	BA	1535	A	C2-N3-C4	17.75	119.48	110.60
22	BA	1545	A	C2-N3-C4	17.75	119.48	110.60
22	BA	471	A	N1-C2-N3	-17.75	120.42	129.30
22	BA	743	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	878	A	N1-C2-N3	-17.75	120.42	129.30
1	AA	635	A	N1-C6-N6	-17.75	107.95	118.60
1	AA	160	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	1247	A	N1-C6-N6	-17.75	107.95	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1871	A	C2-N3-C4	17.75	119.47	110.60
1	AA	468	A	N1-C2-N3	-17.75	120.43	129.30
22	BA	213	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	1413	A	C2-N3-C4	17.75	119.47	110.60
1	AA	250	A	C2-N3-C4	17.74	119.47	110.60
1	AA	53	A	N1-C6-N6	-17.74	107.95	118.60
1	AA	807	A	N1-C6-N6	-17.74	107.95	118.60
1	AA	1346	A	C2-N3-C4	17.74	119.47	110.60
22	BA	917	A	N1-C6-N6	-17.74	107.95	118.60
22	BA	936	A	C2-N3-C4	17.74	119.47	110.60
22	BA	2058	A	C2-N3-C4	17.74	119.47	110.60
54	B7	9	A	C2-N3-C4	17.74	119.47	110.60
22	BA	470	A	N1-C2-N3	-17.74	120.43	129.30
1	AA	411	A	C2-N3-C4	17.74	119.47	110.60
22	BA	920	A	N1-C6-N6	-17.74	107.96	118.60
22	BA	1876	A	N1-C2-N3	-17.74	120.43	129.30
22	BA	2176	A	C2-N3-C4	17.74	119.47	110.60
22	BA	2336	A	C2-N3-C4	17.74	119.47	110.60
22	BA	2813	A	N1-C2-N3	-17.74	120.43	129.30
1	AA	1446	A	N1-C2-N3	-17.73	120.43	129.30
22	BA	572	A	N1-C2-N3	-17.73	120.43	129.30
22	BA	2482	A	N1-C2-N3	-17.73	120.43	129.30
22	BA	2033	A	C2-N3-C4	17.73	119.47	110.60
22	BA	2547	A	N1-C2-N3	-17.73	120.43	129.30
1	AA	782	A	N1-C6-N6	-17.73	107.96	118.60
22	BA	627	A	N1-C6-N6	-17.73	107.96	118.60
22	BA	1301	A	N1-C2-N3	-17.73	120.43	129.30
22	BA	1365	A	C2-N3-C4	17.73	119.47	110.60
22	BA	1722	A	C2-N3-C4	17.73	119.47	110.60
22	BA	1596	A	C2-N3-C4	17.73	119.47	110.60
22	BA	2176	A	N1-C2-N3	-17.73	120.44	129.30
22	BA	2241	A	N1-C2-N3	-17.73	120.44	129.30
22	BA	2809	A	N1-C6-N6	-17.73	107.96	118.60
1	AA	640	A	N1-C2-N3	-17.73	120.44	129.30
22	BA	1490	A	N1-C2-N3	-17.73	120.44	129.30
1	AA	78	A	N1-C6-N6	-17.72	107.97	118.60
22	BA	2513	A	N1-C6-N6	-17.72	107.97	118.60
22	BA	1899	A	N1-C2-N3	-17.72	120.44	129.30
22	BA	2019	A	N1-C6-N6	-17.72	107.97	118.60
1	AA	607	A	N1-C2-N3	-17.72	120.44	129.30
22	BA	504	A	C2-N3-C4	17.72	119.46	110.60
22	BA	2378	A	C2-N3-C4	17.72	119.46	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	103	A	N1-C2-N3	-17.72	120.44	129.30
22	BA	1913	A	N1-C2-N3	-17.72	120.44	129.30
22	BA	1913	A	N1-C6-N6	-17.72	107.97	118.60
22	BA	2459	A	N1-C2-N3	-17.72	120.44	129.30
22	BA	2725	A	C2-N3-C4	17.72	119.46	110.60
55	B8	38	A	C2-N3-C4	17.72	119.46	110.60
1	AA	1179	A	C2-N3-C4	17.71	119.46	110.60
1	AA	1014	A	N1-C2-N3	-17.71	120.44	129.30
1	AA	1092	A	C2-N3-C4	17.71	119.46	110.60
1	AA	1507	A	N1-C2-N3	-17.71	120.44	129.30
22	BA	1749	A	N1-C2-N3	-17.71	120.44	129.30
22	BA	2183	A	N1-C6-N6	-17.71	107.97	118.60
1	AA	655	A	N1-C6-N6	-17.71	107.97	118.60
22	BA	226	A	C2-N3-C4	17.71	119.45	110.60
22	BA	1265	A	N1-C2-N3	-17.71	120.44	129.30
23	BB	66	A	N1-C6-N6	-17.71	107.97	118.60
1	AA	1180	A	N1-C2-N3	-17.71	120.45	129.30
22	BA	718	A	C2-N3-C4	17.71	119.45	110.60
22	BA	718	A	N1-C2-N3	-17.71	120.45	129.30
22	BA	756	A	N1-C2-N3	-17.71	120.45	129.30
22	BA	945	A	N1-C2-N3	-17.71	120.45	129.30
1	AA	831	A	N1-C2-N3	-17.71	120.45	129.30
1	AA	1167	A	C2-N3-C4	17.71	119.45	110.60
22	BA	73	A	C2-N3-C4	17.71	119.45	110.60
1	AA	448	A	C2-N3-C4	17.70	119.45	110.60
1	AA	819	A	C2-N3-C4	17.70	119.45	110.60
1	AA	1275	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	1054	A	C2-N3-C4	17.70	119.45	110.60
22	BA	430	A	C2-N3-C4	17.70	119.45	110.60
22	BA	861	A	N1-C2-N3	-17.70	120.45	129.30
22	BA	49	A	C2-N3-C4	17.70	119.45	110.60
22	BA	1009	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	19	A	N1-C2-N3	-17.70	120.45	129.30
22	BA	91	A	C2-N3-C4	17.70	119.45	110.60
22	BA	322	A	C2-N3-C4	17.70	119.45	110.60
22	BA	722	A	N1-C2-N3	-17.70	120.45	129.30
22	BA	743	A	C2-N3-C4	17.70	119.45	110.60
22	BA	1757	A	N1-C2-N3	-17.70	120.45	129.30
1	AA	139	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	272	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	1665	A	N1-C2-N3	-17.70	120.45	129.30
22	BA	1805	A	N1-C6-N6	-17.70	107.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2725	A	N1-C2-N3	-17.70	120.45	129.30
1	AA	1102	A	N1-C6-N6	-17.69	107.98	118.60
1	AA	279	A	N1-C2-N3	-17.69	120.45	129.30
1	AA	663	A	C2-N3-C4	17.69	119.44	110.60
22	BA	616	A	N1-C2-N3	-17.69	120.46	129.30
1	AA	977	A	N1-C2-N3	-17.69	120.46	129.30
22	BA	1247	A	N1-C2-N3	-17.69	120.46	129.30
1	AA	969	A	C2-N3-C4	17.68	119.44	110.60
22	BA	1433	A	N1-C6-N6	-17.68	107.99	118.60
1	AA	702	A	N1-C6-N6	-17.68	107.99	118.60
1	AA	1021	A	N1-C6-N6	-17.68	107.99	118.60
1	AA	1046	A	N1-C6-N6	-17.68	107.99	118.60
22	BA	603	A	N1-C6-N6	-17.68	107.99	118.60
22	BA	1801	A	N1-C2-N3	-17.68	120.46	129.30
22	BA	233	A	C2-N3-C4	17.68	119.44	110.60
1	AA	172	A	C2-N3-C4	17.68	119.44	110.60
22	BA	196	A	N1-C2-N3	-17.68	120.46	129.30
22	BA	1912	A	C2-N3-C4	17.68	119.44	110.60
22	BA	2322	A	N1-C2-N3	-17.68	120.46	129.30
1	AA	487	A	N1-C6-N6	-17.67	108.00	118.60
22	BA	89	A	N1-C6-N6	-17.67	108.00	118.60
22	BA	980	A	N1-C6-N6	-17.67	108.00	118.60
22	BA	2088	A	N1-C2-N3	-17.67	120.46	129.30
22	BA	492	A	C2-N3-C4	17.67	119.44	110.60
22	BA	633	A	N1-C2-N3	-17.67	120.46	129.30
22	BA	2154	A	N1-C2-N3	-17.67	120.46	129.30
1	AA	547	A	C2-N3-C4	17.67	119.44	110.60
1	AA	1429	A	N1-C2-N3	-17.67	120.47	129.30
22	BA	582	A	N1-C2-N3	-17.67	120.47	129.30
22	BA	2358	A	C2-N3-C4	17.67	119.43	110.60
1	AA	873	A	C2-N3-C4	17.66	119.43	110.60
1	AA	1157	A	N1-C2-N3	-17.66	120.47	129.30
1	AA	1082	A	C2-N3-C4	17.66	119.43	110.60
1	AA	1271	A	N1-C6-N6	-17.66	108.00	118.60
22	BA	73	A	N1-C6-N6	-17.66	108.00	118.60
1	AA	630	A	C2-N3-C4	17.66	119.43	110.60
1	AA	1280	A	N1-C2-N3	-17.66	120.47	129.30
22	BA	1260	A	N1-C2-N3	-17.66	120.47	129.30
22	BA	1321	A	N1-C2-N3	-17.66	120.47	129.30
22	BA	1711	A	C2-N3-C4	17.66	119.43	110.60
22	BA	715	A	C2-N3-C4	17.66	119.43	110.60
22	BA	1014	A	N1-C2-N3	-17.66	120.47	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2660	A	N1-C2-N3	-17.66	120.47	129.30
1	AA	50	A	N1-C6-N6	-17.66	108.01	118.60
1	AA	1531	A	C2-N3-C4	17.66	119.43	110.60
22	BA	2288	A	N1-C6-N6	-17.66	108.01	118.60
23	BB	119	A	N1-C6-N6	-17.66	108.01	118.60
22	BA	1690	A	N1-C2-N3	-17.65	120.47	129.30
1	AA	441	A	N1-C6-N6	-17.65	108.01	118.60
1	AA	702	A	N1-C2-N3	-17.65	120.47	129.30
1	AA	1531	A	N1-C6-N6	-17.65	108.01	118.60
22	BA	2090	A	N1-C2-N3	-17.65	120.47	129.30
22	BA	2346	A	N1-C2-N3	-17.65	120.47	129.30
1	AA	263	A	C2-N3-C4	17.65	119.42	110.60
1	AA	1250	A	N1-C2-N3	-17.65	120.48	129.30
22	BA	1711	A	N1-C2-N3	-17.65	120.48	129.30
22	BA	1505	A	N1-C2-N3	-17.65	120.48	129.30
22	BA	626	A	N1-C2-N3	-17.64	120.48	129.30
22	BA	1610	A	C2-N3-C4	17.64	119.42	110.60
22	BA	1230	A	N1-C6-N6	-17.64	108.01	118.60
22	BA	1609	A	N1-C2-N3	-17.64	120.48	129.30
1	AA	510	A	N1-C6-N6	-17.64	108.02	118.60
1	AA	629	A	N1-C2-N3	-17.64	120.48	129.30
1	AA	1146	A	N1-C6-N6	-17.64	108.02	118.60
1	AA	288	A	N1-C6-N6	-17.64	108.02	118.60
1	AA	499	A	C2-N3-C4	17.64	119.42	110.60
22	BA	1237	A	C2-N3-C4	17.64	119.42	110.60
22	BA	2800	A	C2-N3-C4	17.64	119.42	110.60
22	BA	52	A	N1-C2-N3	-17.64	120.48	129.30
22	BA	256	A	N1-C2-N3	-17.64	120.48	129.30
22	BA	2071	A	C2-N3-C4	17.64	119.42	110.60
1	AA	366	A	C2-N3-C4	17.64	119.42	110.60
1	AA	687	A	C2-N3-C4	17.64	119.42	110.60
1	AA	768	A	C2-N3-C4	17.64	119.42	110.60
1	AA	1044	A	N1-C2-N3	-17.64	120.48	129.30
22	BA	1580	A	N1-C2-N3	-17.64	120.48	129.30
1	AA	139	A	N1-C2-N3	-17.63	120.48	129.30
22	BA	347	A	N1-C2-N3	-17.63	120.48	129.30
22	BA	2388	A	N1-C6-N6	-17.63	108.02	118.60
22	BA	2662	A	N1-C2-N3	-17.63	120.48	129.30
1	AA	452	A	C2-N3-C4	17.63	119.42	110.60
1	AA	572	A	C2-N3-C4	17.63	119.42	110.60
1	AA	1480	A	N1-C2-N3	-17.63	120.48	129.30
22	BA	218	A	N1-C6-N6	-17.63	108.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	466	A	N1-C2-N3	-17.63	120.48	129.30
22	BA	896	A	C2-N3-C4	17.63	119.42	110.60
1	AA	493	A	C2-N3-C4	17.63	119.42	110.60
22	BA	1583	A	C2-N3-C4	17.63	119.42	110.60
1	AA	119	A	C2-N3-C4	17.63	119.42	110.60
1	AA	906	A	N1-C2-N3	-17.63	120.48	129.30
1	AA	1503	A	N1-C2-N3	-17.63	120.48	129.30
22	BA	256	A	N1-C6-N6	-17.63	108.02	118.60
22	BA	504	A	N1-C6-N6	-17.63	108.02	118.60
1	AA	435	A	N1-C2-N3	-17.62	120.49	129.30
22	BA	443	A	N1-C2-N3	-17.62	120.49	129.30
1	AA	195	A	N1-C2-N3	-17.62	120.49	129.30
1	AA	1396	A	N1-C6-N6	-17.62	108.03	118.60
1	AA	1534	A	C2-N3-C4	17.62	119.41	110.60
22	BA	63	A	N1-C2-N3	-17.62	120.49	129.30
22	BA	892	A	N1-C2-N3	-17.62	120.49	129.30
22	BA	2758	A	C2-N3-C4	17.62	119.41	110.60
1	AA	1111	A	N1-C2-N3	-17.62	120.49	129.30
1	AA	1492	A	N1-C6-N6	-17.62	108.03	118.60
1	AA	687	A	N1-C6-N6	-17.62	108.03	118.60
1	AA	574	A	N1-C6-N6	-17.61	108.03	118.60
22	BA	2868	A	N1-C6-N6	-17.61	108.03	118.60
1	AA	907	A	N1-C6-N6	-17.61	108.03	118.60
22	BA	1088	A	N1-C6-N6	-17.61	108.03	118.60
1	AA	109	A	N1-C2-N3	-17.61	120.50	129.30
22	BA	613	A	N1-C2-N3	-17.61	120.50	129.30
22	BA	1890	A	C2-N3-C4	17.61	119.41	110.60
1	AA	298	A	N1-C2-N3	-17.61	120.50	129.30
1	AA	329	A	C2-N3-C4	17.61	119.40	110.60
1	AA	749	A	N1-C2-N3	-17.61	120.50	129.30
1	AA	935	A	N1-C2-N3	-17.61	120.50	129.30
22	BA	2386	A	N1-C2-N3	-17.61	120.50	129.30
1	AA	1480	A	C2-N3-C4	17.61	119.40	110.60
23	BB	52	A	C2-N3-C4	17.61	119.40	110.60
22	BA	734	A	N1-C2-N3	-17.60	120.50	129.30
22	BA	1269	A	N1-C6-N6	-17.60	108.04	118.60
22	BA	2418	A	C2-N3-C4	17.60	119.40	110.60
1	AA	1429	A	N1-C6-N6	-17.60	108.04	118.60
22	BA	1226	A	N1-C2-N3	-17.60	120.50	129.30
55	B8	14	A	N1-C2-N3	-17.60	120.50	129.30
1	AA	8	A	C2-N3-C4	17.60	119.40	110.60
1	AA	495	A	N1-C6-N6	-17.60	108.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	937	A	N1-C6-N6	-17.60	108.04	118.60
22	BA	2425	A	N1-C2-N3	-17.60	120.50	129.30
22	BA	368	A	N1-C2-N3	-17.59	120.50	129.30
22	BA	447	A	C2-N3-C4	17.59	119.40	110.60
22	BA	1027	A	N1-C2-N3	-17.59	120.50	129.30
22	BA	1535	A	N1-C2-N3	-17.59	120.50	129.30
22	BA	1829	A	C2-N3-C4	17.59	119.40	110.60
22	BA	2281	A	N1-C2-N3	-17.59	120.50	129.30
22	BA	1302	A	N1-C2-N3	-17.59	120.50	129.30
1	AA	695	A	N1-C2-N3	-17.59	120.50	129.30
22	BA	83	A	C2-N3-C4	17.59	119.39	110.60
22	BA	345	A	N1-C6-N6	-17.59	108.05	118.60
1	AA	325	A	N1-C6-N6	-17.59	108.05	118.60
1	AA	373	A	C2-N3-C4	17.59	119.39	110.60
1	AA	864	A	N1-C6-N6	-17.59	108.05	118.60
22	BA	522	A	N1-C2-N3	-17.59	120.51	129.30
22	BA	1169	A	N1-C2-N3	-17.59	120.51	129.30
1	AA	1110	A	N1-C2-N3	-17.59	120.51	129.30
22	BA	478	A	N1-C2-N3	-17.59	120.51	129.30
22	BA	2893	A	C2-N3-C4	17.59	119.39	110.60
55	B8	76	A	C2-N3-C4	17.59	119.39	110.60
1	AA	55	A	C2-N3-C4	17.59	119.39	110.60
22	BA	483	A	N1-C6-N6	-17.59	108.05	118.60
22	BA	1385	A	C2-N3-C4	17.59	119.39	110.60
22	BA	2052	A	C2-N3-C4	17.59	119.39	110.60
1	AA	19	A	N1-C6-N6	-17.58	108.05	118.60
1	AA	1188	A	N1-C2-N3	-17.58	120.51	129.30
1	AA	1507	A	C2-N3-C4	17.58	119.39	110.60
22	BA	1689	A	N1-C2-N3	-17.58	120.51	129.30
22	BA	1787	A	N1-C2-N3	-17.58	120.51	129.30
22	BA	2873	A	C2-N3-C4	17.58	119.39	110.60
22	BA	1494	A	C2-N3-C4	17.58	119.39	110.60
22	BA	1553	A	N1-C2-N3	-17.58	120.51	129.30
1	AA	629	A	N1-C6-N6	-17.58	108.05	118.60
22	BA	1020	A	N1-C6-N6	-17.58	108.05	118.60
1	AA	109	A	C2-N3-C4	17.58	119.39	110.60
1	AA	182	A	C2-N3-C4	17.58	119.39	110.60
1	AA	1250	A	C2-N3-C4	17.57	119.39	110.60
22	BA	627	A	C2-N3-C4	17.57	119.39	110.60
22	BA	1126	A	C2-N3-C4	17.57	119.39	110.60
22	BA	1717	A	N1-C2-N3	-17.57	120.51	129.30
22	BA	126	A	C2-N3-C4	17.57	119.39	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2169	A	N1-C2-N3	-17.57	120.51	129.30
1	AA	162	A	C2-N3-C4	17.57	119.39	110.60
1	AA	1081	A	N1-C2-N3	-17.57	120.51	129.30
22	BA	1552	A	N1-C2-N3	-17.57	120.51	129.30
23	BB	108	A	C2-N3-C4	17.57	119.39	110.60
22	BA	2135	A	C2-N3-C4	17.57	119.39	110.60
22	BA	2163	A	C2-N3-C4	17.57	119.39	110.60
22	BA	2577	A	C2-N3-C4	17.57	119.39	110.60
1	AA	1503	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	374	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	614	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	1387	A	C2-N3-C4	17.57	119.38	110.60
22	BA	1566	A	C2-N3-C4	17.57	119.38	110.60
1	AA	1252	A	N1-C2-N3	-17.57	120.52	129.30
22	BA	2114	A	N1-C2-N3	-17.57	120.52	129.30
22	BA	2336	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	706	A	N1-C2-N3	-17.57	120.52	129.30
22	BA	2080	A	N1-C2-N3	-17.57	120.52	129.30
1	AA	80	A	N1-C6-N6	-17.56	108.06	118.60
1	AA	794	A	N1-C2-N3	-17.56	120.52	129.30
22	BA	1470	A	N1-C2-N3	-17.56	120.52	129.30
22	BA	340	A	N1-C2-N3	-17.56	120.52	129.30
1	AA	466	A	N1-C2-N3	-17.56	120.52	129.30
1	AA	532	A	N1-C6-N6	-17.56	108.06	118.60
22	BA	2247	A	N1-C6-N6	-17.56	108.06	118.60
1	AA	602	A	N1-C6-N6	-17.56	108.06	118.60
22	BA	1508	A	C2-N3-C4	17.55	119.38	110.60
22	BA	2117	A	C2-N3-C4	17.55	119.38	110.60
1	AA	1394	A	N1-C6-N6	-17.55	108.07	118.60
22	BA	1366	A	N1-C2-N3	-17.55	120.52	129.30
22	BA	743	A	N1-C2-N3	-17.55	120.53	129.30
22	BA	975	A	C2-N3-C4	17.55	119.38	110.60
1	AA	729	A	C2-N3-C4	17.55	119.38	110.60
23	BB	39	A	C2-N3-C4	17.55	119.37	110.60
1	AA	535	A	C2-N3-C4	17.55	119.37	110.60
22	BA	917	A	C2-N3-C4	17.55	119.37	110.60
1	AA	303	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	1144	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	1802	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	1014	A	C2-N3-C4	17.54	119.37	110.60
22	BA	1073	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	1077	A	C2-N3-C4	17.54	119.37	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1735	A	N1-C6-N6	-17.54	108.07	118.60
22	BA	2766	A	N1-C6-N6	-17.54	108.08	118.60
22	BA	820	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	1284	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	2154	A	N1-C6-N6	-17.54	108.08	118.60
1	AA	1311	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	2705	A	N1-C6-N6	-17.54	108.08	118.60
22	BA	2900	A	N1-C6-N6	-17.54	108.08	118.60
1	AA	309	A	N1-C6-N6	-17.54	108.08	118.60
22	BA	2191	A	C2-N3-C4	17.54	119.37	110.60
1	AA	1238	A	N1-C2-N3	-17.53	120.53	129.30
1	AA	1408	A	N1-C6-N6	-17.53	108.08	118.60
22	BA	751	A	C2-N3-C4	17.53	119.37	110.60
1	AA	845	A	N1-C2-N3	-17.53	120.53	129.30
1	AA	1374	A	N1-C2-N3	-17.53	120.53	129.30
1	AA	51	A	C2-N3-C4	17.53	119.36	110.60
22	BA	1877	A	C2-N3-C4	17.53	119.36	110.60
22	BA	1889	A	N1-C2-N3	-17.53	120.53	129.30
1	AA	10	A	N1-C6-N6	-17.53	108.08	118.60
22	BA	1254	A	N1-C2-N3	-17.53	120.54	129.30
22	BA	1608	A	N1-C2-N3	-17.53	120.54	129.30
1	AA	635	A	N1-C2-N3	-17.52	120.54	129.30
1	AA	1363	A	N1-C6-N6	-17.52	108.08	118.60
22	BA	1155	A	C2-N3-C4	17.52	119.36	110.60
22	BA	1373	A	N1-C2-N3	-17.52	120.54	129.30
1	AA	1274	A	N1-C2-N3	-17.52	120.54	129.30
22	BA	1634	A	C2-N3-C4	17.52	119.36	110.60
22	BA	1746	A	C2-N3-C4	17.52	119.36	110.60
22	BA	2309	A	C2-N3-C4	17.52	119.36	110.60
22	BA	2333	A	N1-C2-N3	-17.52	120.54	129.30
1	AA	51	A	N1-C2-N3	-17.52	120.54	129.30
1	AA	510	A	C2-N3-C4	17.52	119.36	110.60
1	AA	1483	A	N1-C2-N3	-17.52	120.54	129.30
22	BA	144	A	N1-C2-N3	-17.52	120.54	129.30
22	BA	2531	A	C2-N3-C4	17.52	119.36	110.60
1	AA	1534	A	N1-C2-N3	-17.52	120.54	129.30
1	AA	1287	A	N1-C2-N3	-17.52	120.54	129.30
1	AA	33	A	N1-C2-N3	-17.51	120.54	129.30
22	BA	104	A	C2-N3-C4	17.51	119.36	110.60
22	BA	1048	A	N1-C2-N3	-17.51	120.54	129.30
22	BA	1918	A	N1-C2-N3	-17.51	120.54	129.30
22	BA	142	A	N1-C2-N3	-17.51	120.54	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1150	A	N1-C2-N3	-17.51	120.55	129.30
1	AA	1374	A	N1-C6-N6	-17.51	108.09	118.60
22	BA	19	A	C2-N3-C4	17.51	119.36	110.60
22	BA	1586	A	N1-C2-N3	-17.51	120.55	129.30
1	AA	913	A	C2-N3-C4	17.51	119.35	110.60
1	AA	1441	A	C2-N3-C4	17.51	119.35	110.60
23	BB	46	A	N1-C2-N3	-17.51	120.55	129.30
1	AA	1093	A	N1-C2-N3	-17.51	120.55	129.30
1	AA	1437	A	C2-N3-C4	17.51	119.35	110.60
23	BB	46	A	C2-N3-C4	17.51	119.35	110.60
1	AA	496	A	N1-C6-N6	-17.51	108.10	118.60
1	AA	609	A	N1-C6-N6	-17.51	108.10	118.60
1	AA	946	A	N1-C2-N3	-17.50	120.55	129.30
1	AA	1476	A	N1-C2-N3	-17.50	120.55	129.30
22	BA	1590	A	C2-N3-C4	17.50	119.35	110.60
22	BA	2169	A	C2-N3-C4	17.50	119.35	110.60
22	BA	2171	A	N1-C6-N6	-17.50	108.10	118.60
22	BA	2679	A	N1-C2-N3	-17.50	120.55	129.30
22	BA	439	A	N1-C6-N6	-17.50	108.10	118.60
22	BA	507	A	N1-C6-N6	-17.50	108.10	118.60
1	AA	845	A	C2-N3-C4	17.50	119.35	110.60
22	BA	2530	A	C2-N3-C4	17.50	119.35	110.60
1	AA	539	A	N1-C2-N3	-17.50	120.55	129.30
22	BA	368	A	C2-N3-C4	17.50	119.35	110.60
1	AA	167	A	N1-C6-N6	-17.50	108.10	118.60
1	AA	901	A	C2-N3-C4	17.50	119.35	110.60
1	AA	1130	A	C2-N3-C4	17.50	119.35	110.60
22	BA	654	A	N1-C2-N3	-17.50	120.55	129.30
22	BA	2097	A	N1-C2-N3	-17.50	120.55	129.30
1	AA	320	A	N1-C2-N3	-17.49	120.55	129.30
1	AA	382	A	N1-C2-N3	-17.49	120.55	129.30
1	AA	1055	A	N1-C2-N3	-17.49	120.55	129.30
1	AA	1468	A	N1-C2-N3	-17.49	120.55	129.30
1	AA	815	A	N1-C2-N3	-17.49	120.55	129.30
1	AA	1169	A	N1-C2-N3	-17.49	120.55	129.30
22	BA	1095	A	N1-C2-N3	-17.49	120.55	129.30
22	BA	1308	A	N1-C2-N3	-17.49	120.55	129.30
1	AA	33	A	C2-N3-C4	17.49	119.34	110.60
1	AA	728	A	N1-C2-N3	-17.49	120.56	129.30
22	BA	1746	A	N1-C6-N6	-17.49	108.11	118.60
1	AA	329	A	N1-C6-N6	-17.49	108.11	118.60
1	AA	546	A	N1-C2-N3	-17.49	120.56	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1126	A	N1-C2-N3	-17.49	120.56	129.30
1	AA	1324	A	N1-C6-N6	-17.49	108.11	118.60
22	BA	1634	A	N1-C2-N3	-17.49	120.56	129.30
22	BA	2270	A	C2-N3-C4	17.49	119.34	110.60
22	BA	2418	A	N1-C2-N3	-17.49	120.56	129.30
22	BA	412	A	C2-N3-C4	17.48	119.34	110.60
22	BA	1014	A	N1-C6-N6	-17.48	108.11	118.60
1	AA	1146	A	C2-N3-C4	17.48	119.34	110.60
1	AA	1433	A	N1-C2-N3	-17.48	120.56	129.30
22	BA	1553	A	C2-N3-C4	17.48	119.34	110.60
1	AA	532	A	N1-C2-N3	-17.48	120.56	129.30
1	AA	914	A	N1-C6-N6	-17.48	108.11	118.60
22	BA	1494	A	N1-C6-N6	-17.48	108.11	118.60
22	BA	1664	A	C2-N3-C4	17.48	119.34	110.60
1	AA	441	A	N1-C2-N3	-17.48	120.56	129.30
22	BA	979	A	N1-C2-N3	-17.48	120.56	129.30
22	BA	2879	A	N1-C2-N3	-17.48	120.56	129.30
22	BA	1876	A	C2-N3-C4	17.47	119.34	110.60
22	BA	470	A	C2-N3-C4	17.47	119.33	110.60
22	BA	1029	A	N1-C2-N3	-17.47	120.56	129.30
22	BA	1237	A	N1-C6-N6	-17.47	108.12	118.60
22	BA	614	A	C2-N3-C4	17.47	119.33	110.60
22	BA	1419	A	C2-N3-C4	17.47	119.33	110.60
1	AA	430	A	N1-C6-N6	-17.47	108.12	118.60
1	AA	1256	A	N1-C6-N6	-17.47	108.12	118.60
1	AA	1441	A	N1-C6-N6	-17.47	108.12	118.60
22	BA	1307	A	N1-C2-N3	-17.47	120.57	129.30
22	BA	2358	A	N1-C2-N3	-17.47	120.57	129.30
1	AA	794	A	C2-N3-C4	17.46	119.33	110.60
1	AA	139	A	C2-N3-C4	17.46	119.33	110.60
22	BA	449	A	N1-C6-N6	-17.46	108.12	118.60
22	BA	1780	A	N1-C6-N6	-17.46	108.12	118.60
1	AA	715	A	N1-C6-N6	-17.46	108.12	118.60
22	BA	49	A	N1-C2-N3	-17.46	120.57	129.30
22	BA	2274	A	N1-C2-N3	-17.46	120.57	129.30
22	BA	2412	A	N1-C2-N3	-17.46	120.57	129.30
1	AA	65	A	C2-N3-C4	17.46	119.33	110.60
1	AA	969	A	N1-C2-N3	-17.46	120.57	129.30
22	BA	354	A	C2-N3-C4	17.46	119.33	110.60
22	BA	1900	A	N1-C6-N6	-17.46	108.13	118.60
22	BA	2513	A	N1-C2-N3	-17.46	120.57	129.30
1	AA	681	A	N1-C2-N3	-17.45	120.57	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1216	A	C2-N3-C4	17.45	119.33	110.60
1	AA	1502	A	C2-N3-C4	17.45	119.33	110.60
22	BA	1084	A	C2-N3-C4	17.45	119.33	110.60
1	AA	298	A	N1-C6-N6	-17.45	108.13	118.60
1	AA	712	A	N1-C6-N6	-17.45	108.13	118.60
22	BA	1241	A	C2-N3-C4	17.45	119.33	110.60
1	AA	1151	A	N1-C2-N3	-17.45	120.58	129.30
22	BA	616	A	N1-C6-N6	-17.45	108.13	118.60
22	BA	2135	A	N1-C2-N3	-17.44	120.58	129.30
22	BA	1040	A	N1-C2-N3	-17.44	120.58	129.30
1	AA	1236	A	N1-C2-N3	-17.44	120.58	129.30
22	BA	182	A	C2-N3-C4	17.44	119.32	110.60
22	BA	2142	A	N1-C6-N6	-17.44	108.14	118.60
22	BA	2733	A	C2-N3-C4	17.44	119.32	110.60
1	AA	1252	A	N1-C6-N6	-17.44	108.14	118.60
22	BA	1477	A	N1-C6-N6	-17.44	108.14	118.60
22	BA	1503	A	C2-N3-C4	17.44	119.32	110.60
1	AA	759	A	N1-C6-N6	-17.44	108.14	118.60
1	AA	1196	A	C2-N3-C4	17.44	119.32	110.60
22	BA	1890	A	N1-C2-N3	-17.44	120.58	129.30
1	AA	1176	A	N1-C2-N3	-17.43	120.58	129.30
22	BA	751	A	N1-C2-N3	-17.43	120.58	129.30
1	AA	430	A	C2-N3-C4	17.43	119.32	110.60
1	AA	1216	A	N1-C6-N6	-17.43	108.14	118.60
22	BA	374	A	N1-C2-N3	-17.43	120.58	129.30
22	BA	1652	A	C2-N3-C4	17.43	119.32	110.60
1	AA	71	A	C2-N3-C4	17.43	119.31	110.60
1	AA	937	A	N1-C2-N3	-17.43	120.59	129.30
1	AA	1012	A	N1-C6-N6	-17.43	108.14	118.60
22	BA	1701	A	N1-C2-N3	-17.43	120.59	129.30
22	BA	1794	A	N1-C6-N6	-17.43	108.14	118.60
22	BA	2058	A	N1-C6-N6	-17.43	108.14	118.60
22	BA	2860	A	C2-N3-C4	17.43	119.31	110.60
1	AA	600	A	C2-N3-C4	17.42	119.31	110.60
22	BA	63	A	C2-N3-C4	17.42	119.31	110.60
22	BA	2662	A	C2-N3-C4	17.42	119.31	110.60
1	AA	681	A	C2-N3-C4	17.42	119.31	110.60
1	AA	1271	A	C2-N3-C4	17.42	119.31	110.60
23	BB	15	A	N1-C6-N6	-17.42	108.15	118.60
1	AA	964	A	N1-C2-N3	-17.42	120.59	129.30
22	BA	1077	A	N1-C2-N3	-17.42	120.59	129.30
22	BA	1304	A	N1-C6-N6	-17.42	108.15	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1690	A	C2-N3-C4	17.42	119.31	110.60
22	BA	2733	A	N1-C2-N3	-17.42	120.59	129.30
22	BA	844	A	N1-C2-N3	-17.42	120.59	129.30
22	BA	2327	A	N1-C6-N6	-17.42	108.15	118.60
22	BA	2333	A	C2-N3-C4	17.42	119.31	110.60
1	AA	873	A	N1-C6-N6	-17.41	108.15	118.60
22	BA	632	A	C2-N3-C4	17.41	119.31	110.60
1	AA	3	A	N1-C6-N6	-17.41	108.15	118.60
1	AA	759	A	C2-N3-C4	17.41	119.31	110.60
22	BA	219	A	N1-C6-N6	-17.41	108.15	118.60
22	BA	1433	A	N1-C2-N3	-17.41	120.59	129.30
22	BA	2753	A	C2-N3-C4	17.41	119.31	110.60
22	BA	384	A	N1-C6-N6	-17.41	108.15	118.60
22	BA	1302	A	N1-C6-N6	-17.41	108.15	118.60
22	BA	2163	A	N1-C2-N3	-17.41	120.59	129.30
1	AA	499	A	N1-C2-N3	-17.41	120.60	129.30
1	AA	1363	A	N1-C2-N3	-17.41	120.59	129.30
22	BA	38	A	N1-C6-N6	-17.41	108.16	118.60
1	AA	143	A	N1-C2-N3	-17.41	120.60	129.30
22	BA	829	A	C2-N3-C4	17.41	119.30	110.60
22	BA	753	A	N1-C6-N6	-17.40	108.16	118.60
1	AA	1055	A	C2-N3-C4	17.40	119.30	110.60
22	BA	1431	A	N1-C6-N6	-17.40	108.16	118.60
55	B8	59	A	N1-C2-N3	-17.40	120.60	129.30
22	BA	960	A	C2-N3-C4	17.40	119.30	110.60
22	BA	2270	A	N1-C2-N3	-17.40	120.60	129.30
1	AA	1169	A	C2-N3-C4	17.40	119.30	110.60
1	AA	1408	A	N1-C2-N3	-17.40	120.60	129.30
22	BA	127	A	C2-N3-C4	17.40	119.30	110.60
22	BA	471	A	N1-C6-N6	-17.40	108.16	118.60
1	AA	574	A	C2-N3-C4	17.39	119.30	110.60
1	AA	1150	A	C2-N3-C4	17.39	119.30	110.60
22	BA	2158	A	N1-C2-N3	-17.39	120.60	129.30
22	BA	2412	A	C2-N3-C4	17.39	119.30	110.60
22	BA	2602	A	C2-N3-C4	17.39	119.30	110.60
22	BA	2247	A	N1-C2-N3	-17.39	120.61	129.30
22	BA	1069	A	C2-N3-C4	17.39	119.29	110.60
22	BA	2158	A	C2-N3-C4	17.39	119.29	110.60
22	BA	217	A	N1-C2-N3	-17.38	120.61	129.30
22	BA	928	A	N1-C2-N3	-17.38	120.61	129.30
22	BA	1877	A	N1-C2-N3	-17.38	120.61	129.30
22	BA	2317	A	N1-C2-N3	-17.38	120.61	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2386	A	C2-N3-C4	17.38	119.29	110.60
22	BA	94	A	N1-C2-N3	-17.38	120.61	129.30
22	BA	1321	A	C2-N3-C4	17.38	119.29	110.60
22	BA	1590	A	N1-C6-N6	-17.38	108.17	118.60
23	BB	73	A	N1-C6-N6	-17.38	108.17	118.60
1	AA	1431	A	C2-N3-C4	17.38	119.29	110.60
22	BA	2031	A	N1-C6-N6	-17.38	108.17	118.60
1	AA	246	A	C2-N3-C4	17.37	119.29	110.60
1	AA	640	A	N1-C6-N6	-17.37	108.18	118.60
22	BA	95	A	N1-C2-N3	-17.37	120.61	129.30
1	AA	816	A	N1-C6-N6	-17.37	108.18	118.60
1	AA	430	A	N1-C2-N3	-17.36	120.62	129.30
22	BA	2820	A	N1-C6-N6	-17.36	108.18	118.60
22	BA	362	A	N1-C2-N3	-17.36	120.62	129.30
22	BA	574	A	N1-C6-N6	-17.36	108.18	118.60
22	BA	2101	A	N1-C2-N3	-17.36	120.62	129.30
1	AA	356	A	N1-C2-N3	-17.36	120.62	129.30
22	BA	1496	A	N1-C6-N6	-17.36	108.19	118.60
22	BA	2009	A	N1-C6-N6	-17.36	108.19	118.60
1	AA	819	A	N1-C2-N3	-17.36	120.62	129.30
22	BA	167	A	N1-C2-N3	-17.36	120.62	129.30
1	AA	101	A	N1-C2-N3	-17.36	120.62	129.30
1	AA	1483	A	C2-N3-C4	17.36	119.28	110.60
22	BA	1635	A	N1-C6-N6	-17.36	108.19	118.60
23	BB	58	A	C2-N3-C4	17.36	119.28	110.60
22	BA	1913	A	C2-N3-C4	17.36	119.28	110.60
22	BA	715	A	N1-C6-N6	-17.35	108.19	118.60
22	BA	95	A	C2-N3-C4	17.35	119.28	110.60
22	BA	1365	A	N1-C2-N3	-17.35	120.63	129.30
22	BA	1735	A	N1-C2-N3	-17.35	120.63	129.30
22	BA	216	A	N1-C2-N3	-17.35	120.63	129.30
22	BA	2267	A	N1-C2-N3	-17.35	120.63	129.30
1	AA	1151	A	N1-C6-N6	-17.34	108.19	118.60
22	BA	1088	A	N1-C2-N3	-17.34	120.63	129.30
22	BA	1735	A	C2-N3-C4	17.34	119.27	110.60
22	BA	1205	A	C2-N3-C4	17.34	119.27	110.60
22	BA	1353	A	N1-C2-N3	-17.34	120.63	129.30
1	AA	1082	A	N1-C2-N3	-17.34	120.63	129.30
22	BA	218	A	N1-C2-N3	-17.34	120.63	129.30
22	BA	2328	A	C2-N3-C4	17.34	119.27	110.60
1	AA	1456	A	C2-N3-C4	17.34	119.27	110.60
22	BA	1194	A	N1-C2-N3	-17.34	120.63	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	B8	26	A	N1-C6-N6	-17.34	108.20	118.60
22	BA	1579	A	N1-C2-N3	-17.33	120.63	129.30
22	BA	1046	A	C2-N3-C4	17.33	119.27	110.60
22	BA	1272	A	C2-N3-C4	17.33	119.27	110.60
22	BA	1276	A	N1-C2-N3	-17.33	120.64	129.30
1	AA	1000	A	N1-C6-N6	-17.33	108.20	118.60
22	BA	2851	A	C2-N3-C4	17.33	119.26	110.60
1	AA	648	A	N1-C2-N3	-17.33	120.64	129.30
1	AA	712	A	N1-C2-N3	-17.32	120.64	129.30
22	BA	878	A	C2-N3-C4	17.32	119.26	110.60
22	BA	1801	A	N1-C6-N6	-17.32	108.21	118.60
1	AA	815	A	C2-N3-C4	17.32	119.26	110.60
22	BA	2009	A	N1-C2-N3	-17.32	120.64	129.30
1	AA	702	A	C2-N3-C4	17.32	119.26	110.60
1	AA	1456	A	N1-C2-N3	-17.32	120.64	129.30
1	AA	579	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	324	A	N1-C2-N3	-17.32	120.64	129.30
1	AA	1508	A	C2-N3-C4	17.32	119.26	110.60
22	BA	1151	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	1508	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	1678	A	N1-C6-N6	-17.31	108.21	118.60
22	BA	2126	A	C2-N3-C4	17.31	119.26	110.60
1	AA	602	A	N1-C2-N3	-17.31	120.64	129.30
1	AA	790	A	C2-N3-C4	17.31	119.25	110.60
22	BA	83	A	N1-C2-N3	-17.31	120.64	129.30
22	BA	730	A	C2-N3-C4	17.31	119.25	110.60
22	BA	753	A	N1-C2-N3	-17.31	120.65	129.30
22	BA	1528	A	N1-C2-N3	-17.31	120.64	129.30
22	BA	749	A	N1-C2-N3	-17.31	120.65	129.30
22	BA	819	A	N1-C2-N3	-17.31	120.65	129.30
1	AA	195	A	C2-N3-C4	17.31	119.25	110.60
22	BA	2378	A	N1-C2-N3	-17.31	120.65	129.30
1	AA	1254	A	N1-C2-N3	-17.30	120.65	129.30
22	BA	2654	A	C2-N3-C4	17.30	119.25	110.60
1	AA	338	A	C2-N3-C4	17.30	119.25	110.60
22	BA	917	A	N1-C2-N3	-17.30	120.65	129.30
22	BA	1532	A	C2-N3-C4	17.30	119.25	110.60
22	BA	1866	A	N1-C2-N3	-17.30	120.65	129.30
1	AA	192	A	N1-C2-N3	-17.30	120.65	129.30
22	BA	900	A	N1-C2-N3	-17.30	120.65	129.30
22	BA	1711	A	N1-C6-N6	-17.30	108.22	118.60
1	AA	1493	A	N1-C2-N3	-17.30	120.65	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	477	A	C2-N3-C4	17.30	119.25	110.60
22	BA	1871	A	N1-C6-N6	-17.30	108.22	118.60
22	BA	2434	A	N1-C2-N3	-17.30	120.65	129.30
22	BA	1590	A	N1-C2-N3	-17.30	120.65	129.30
22	BA	2820	A	N1-C2-N3	-17.30	120.65	129.30
22	BA	156	A	N1-C2-N3	-17.29	120.65	129.30
1	AA	431	A	C2-N3-C4	17.29	119.25	110.60
1	AA	860	A	C2-N3-C4	17.29	119.25	110.60
22	BA	1591	A	N1-C6-N6	-17.29	108.23	118.60
22	BA	1746	A	N1-C2-N3	-17.29	120.65	129.30
1	AA	28	A	N1-C2-N3	-17.29	120.66	129.30
1	AA	784	A	N1-C6-N6	-17.29	108.23	118.60
1	AA	1163	A	N1-C2-N3	-17.29	120.66	129.30
1	AA	1152	A	N1-C2-N3	-17.29	120.66	129.30
1	AA	1350	A	N1-C2-N3	-17.29	120.66	129.30
1	AA	1130	A	N1-C2-N3	-17.29	120.66	129.30
22	BA	227	A	N1-C6-N6	-17.29	108.23	118.60
1	AA	263	A	N1-C2-N3	-17.29	120.66	129.30
1	AA	327	A	N1-C6-N6	-17.28	108.23	118.60
1	AA	1492	A	N1-C2-N3	-17.28	120.66	129.30
22	BA	1528	A	C2-N3-C4	17.28	119.24	110.60
1	AA	938	A	N1-C2-N3	-17.28	120.66	129.30
22	BA	1815	A	N1-C6-N6	-17.28	108.23	118.60
1	AA	716	A	C2-N3-C4	17.28	119.24	110.60
22	BA	1328	A	N1-C2-N3	-17.28	120.66	129.30
22	BA	1854	A	N1-C2-N3	-17.28	120.66	129.30
1	AA	1468	A	C2-N3-C4	17.28	119.24	110.60
1	AA	554	A	C2-N3-C4	17.28	119.24	110.60
1	AA	1236	A	N1-C6-N6	-17.28	108.23	118.60
22	BA	1054	A	N1-C6-N6	-17.28	108.23	118.60
22	BA	2426	A	N1-C6-N6	-17.28	108.23	118.60
22	BA	1616	A	N1-C2-N3	-17.28	120.66	129.30
22	BA	472	A	N1-C2-N3	-17.27	120.66	129.30
1	AA	1465	A	N1-C6-N6	-17.27	108.24	118.60
22	BA	2814	A	N1-C6-N6	-17.27	108.24	118.60
22	BA	1269	A	C2-N3-C4	17.27	119.23	110.60
22	BA	1899	A	C2-N3-C4	17.27	119.23	110.60
22	BA	374	A	C2-N3-C4	17.27	119.23	110.60
22	BA	2278	A	N1-C2-N3	-17.27	120.67	129.30
22	BA	2872	A	C2-N3-C4	17.27	119.23	110.60
22	BA	911	A	N1-C2-N3	-17.27	120.67	129.30
22	BA	505	A	C2-N3-C4	17.27	119.23	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	526	A	N1-C2-N3	-17.27	120.67	129.30
22	BA	668	A	N1-C6-N6	-17.27	108.24	118.60
22	BA	2205	A	N1-C2-N3	-17.27	120.67	129.30
1	AA	1357	A	C2-N3-C4	17.26	119.23	110.60
22	BA	2054	A	N1-C6-N6	-17.26	108.24	118.60
22	BA	2792	A	N1-C6-N6	-17.26	108.24	118.60
22	BA	152	A	N1-C2-N3	-17.26	120.67	129.30
22	BA	2284	A	N1-C6-N6	-17.26	108.24	118.60
22	BA	1040	A	C2-N3-C4	17.26	119.23	110.60
22	BA	1919	A	N1-C2-N3	-17.26	120.67	129.30
1	AA	1101	A	C2-N3-C4	17.26	119.23	110.60
22	BA	1532	A	N1-C6-N6	-17.26	108.25	118.60
22	BA	1393	A	N1-C6-N6	-17.25	108.25	118.60
22	BA	2670	A	C2-N3-C4	17.25	119.23	110.60
1	AA	1368	A	N1-C2-N3	-17.25	120.67	129.30
23	BB	50	A	N1-C6-N6	-17.25	108.25	118.60
1	AA	1418	A	C2-N3-C4	17.25	119.22	110.60
22	BA	1977	A	C2-N3-C4	17.25	119.22	110.60
22	BA	2037	A	N1-C2-N3	-17.25	120.68	129.30
22	BA	1745	A	N1-C6-N6	-17.24	108.25	118.60
22	BA	1953	A	N1-C2-N3	-17.24	120.68	129.30
22	BA	118	A	N1-C6-N6	-17.24	108.26	118.60
22	BA	482	A	C2-N3-C4	17.24	119.22	110.60
22	BA	2886	A	C2-N3-C4	17.24	119.22	110.60
1	AA	298	A	C2-N3-C4	17.23	119.22	110.60
22	BA	471	A	C2-N3-C4	17.23	119.22	110.60
22	BA	472	A	C2-N3-C4	17.23	119.22	110.60
22	BA	226	A	N1-C2-N3	-17.23	120.68	129.30
22	BA	2037	A	N1-C6-N6	-17.23	108.26	118.60
22	BA	2821	A	N1-C6-N6	-17.23	108.26	118.60
22	BA	53	A	N1-C6-N6	-17.23	108.26	118.60
55	B8	21	A	N1-C6-N6	-17.23	108.26	118.60
1	AA	946	A	N1-C6-N6	-17.23	108.26	118.60
1	AA	1531	A	N1-C2-N3	-17.23	120.69	129.30
22	BA	348	A	N1-C2-N3	-17.23	120.69	129.30
22	BA	1403	A	N1-C2-N3	-17.22	120.69	129.30
22	BA	1572	A	N1-C6-N6	-17.22	108.27	118.60
1	AA	1503	A	C2-N3-C4	17.22	119.21	110.60
22	BA	844	A	N1-C6-N6	-17.22	108.27	118.60
22	BA	2435	A	N1-C2-N3	-17.22	120.69	129.30
1	AA	373	A	N1-C6-N6	-17.22	108.27	118.60
22	BA	223	A	C2-N3-C4	17.22	119.21	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1000	A	N1-C2-N3	-17.21	120.69	129.30
22	BA	1054	A	N1-C2-N3	-17.21	120.69	129.30
22	BA	1213	A	N1-C2-N3	-17.21	120.69	129.30
1	AA	1227	A	N1-C2-N3	-17.21	120.69	129.30
22	BA	1502	A	N1-C6-N6	-17.21	108.27	118.60
22	BA	2700	A	N1-C2-N3	-17.21	120.69	129.30
22	BA	1783	A	N1-C6-N6	-17.21	108.28	118.60
1	AA	716	A	N1-C6-N6	-17.21	108.28	118.60
22	BA	626	A	C2-N3-C4	17.21	119.20	110.60
22	BA	196	A	N1-C6-N6	-17.20	108.28	118.60
22	BA	272	A	N1-C2-N3	-17.20	120.70	129.30
1	AA	228	A	C2-N3-C4	17.20	119.20	110.60
1	AA	389	A	N1-C2-N3	-17.20	120.70	129.30
22	BA	1981	A	C2-N3-C4	17.20	119.20	110.60
22	BA	1304	A	C2-N3-C4	17.20	119.20	110.60
1	AA	959	A	C2-N3-C4	17.20	119.20	110.60
22	BA	668	A	C2-N3-C4	17.20	119.20	110.60
22	BA	721	A	N1-C6-N6	-17.20	108.28	118.60
22	BA	945	A	C2-N3-C4	17.20	119.20	110.60
22	BA	2082	A	C2-N3-C4	17.20	119.20	110.60
22	BA	909	A	N1-C6-N6	-17.20	108.28	118.60
22	BA	182	A	N1-C6-N6	-17.19	108.28	118.60
1	AA	807	A	C2-N3-C4	17.19	119.19	110.60
1	AA	807	A	N1-C2-N3	-17.19	120.70	129.30
22	BA	2267	A	N1-C6-N6	-17.19	108.29	118.60
1	AA	994	A	N1-C2-N3	-17.19	120.71	129.30
1	AA	199	A	N1-C6-N6	-17.19	108.29	118.60
1	AA	648	A	N1-C6-N6	-17.18	108.29	118.60
23	BB	45	A	N1-C2-N3	-17.18	120.71	129.30
22	BA	2432	A	C2-N3-C4	17.18	119.19	110.60
22	BA	2850	A	N1-C2-N3	-17.18	120.71	129.30
1	AA	181	A	C2-N3-C4	17.18	119.19	110.60
1	AA	655	A	N1-C2-N3	-17.18	120.71	129.30
1	AA	329	A	N1-C2-N3	-17.17	120.71	129.30
22	BA	2534	A	N1-C6-N6	-17.17	108.30	118.60
1	AA	1197	A	N1-C2-N3	-17.17	120.72	129.30
22	BA	2052	A	N1-C2-N3	-17.17	120.71	129.30
1	AA	583	A	N1-C2-N3	-17.17	120.72	129.30
1	AA	371	A	C2-N3-C4	17.17	119.18	110.60
22	BA	2033	A	N1-C2-N3	-17.17	120.72	129.30
23	BB	57	A	N1-C2-N3	-17.17	120.72	129.30
22	BA	2227	A	N1-C2-N3	-17.17	120.72	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1866	A	C2-N3-C4	17.16	119.18	110.60
1	AA	579	A	N1-C2-N3	-17.16	120.72	129.30
1	AA	918	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	155	A	N1-C6-N6	-17.16	108.30	118.60
22	BA	309	A	C2-N3-C4	17.16	119.18	110.60
22	BA	2335	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	2340	A	N1-C6-N6	-17.16	108.30	118.60
1	AA	1306	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	480	A	N1-C2-N3	-17.16	120.72	129.30
1	AA	371	A	N1-C6-N6	-17.16	108.31	118.60
22	BA	1780	A	C2-N3-C4	17.16	119.18	110.60
1	AA	959	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	104	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	2019	A	N1-C2-N3	-17.15	120.72	129.30
1	AA	1105	A	N1-C6-N6	-17.15	108.31	118.60
22	BA	792	A	C2-N3-C4	17.14	119.17	110.60
22	BA	2094	A	N1-C2-N3	-17.14	120.73	129.30
1	AA	746	A	N1-C6-N6	-17.14	108.31	118.60
1	AA	50	A	C2-N3-C4	17.14	119.17	110.60
1	AA	649	A	N1-C6-N6	-17.14	108.32	118.60
1	AA	1219	A	N1-C2-N3	-17.14	120.73	129.30
22	BA	2381	A	N1-C6-N6	-17.13	108.32	118.60
22	BA	947	A	N1-C2-N3	-17.13	120.73	129.30
22	BA	1952	A	N1-C6-N6	-17.13	108.32	118.60
1	AA	1437	A	N1-C6-N6	-17.13	108.32	118.60
22	BA	1010	A	C2-N3-C4	17.13	119.17	110.60
22	BA	1080	A	N1-C2-N3	-17.13	120.73	129.30
22	BA	2727	A	N1-C2-N3	-17.13	120.74	129.30
1	AA	718	A	N1-C2-N3	-17.13	120.74	129.30
1	AA	649	A	C2-N3-C4	17.12	119.16	110.60
1	AA	1012	A	N1-C2-N3	-17.12	120.74	129.30
22	BA	362	A	C2-N3-C4	17.12	119.16	110.60
1	AA	716	A	N1-C2-N3	-17.12	120.74	129.30
22	BA	2184	A	N1-C2-N3	-17.12	120.74	129.30
22	BA	6	A	N1-C2-N3	-17.12	120.74	129.30
1	AA	648	A	C2-N3-C4	17.12	119.16	110.60
1	AA	1306	A	N1-C6-N6	-17.12	108.33	118.60
22	BA	2407	A	C2-N3-C4	17.12	119.16	110.60
1	AA	196	A	C2-N3-C4	17.11	119.16	110.60
22	BA	412	A	N1-C6-N6	-17.11	108.33	118.60
22	BA	1938	A	N1-C2-N3	-17.11	120.74	129.30
22	BA	2534	A	C2-N3-C4	17.11	119.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	655	A	C2-N3-C4	17.11	119.16	110.60
22	BA	1785	A	C2-N3-C4	17.11	119.16	110.60
22	BA	2886	A	N1-C6-N6	-17.11	108.33	118.60
22	BA	1274	A	N1-C6-N6	-17.11	108.33	118.60
1	AA	363	A	N1-C2-N3	-17.11	120.75	129.30
22	BA	428	A	C2-N3-C4	17.11	119.15	110.60
22	BA	1469	A	N1-C2-N3	-17.11	120.75	129.30
1	AA	1163	A	N1-C6-N6	-17.10	108.34	118.60
22	BA	282	A	C2-N3-C4	17.10	119.15	110.60
22	BA	2274	A	C2-N3-C4	17.10	119.15	110.60
22	BA	172	A	N1-C2-N3	-17.10	120.75	129.30
22	BA	1433	A	C2-N3-C4	17.09	119.15	110.60
22	BA	156	A	N1-C6-N6	-17.09	108.34	118.60
1	AA	1324	A	N1-C2-N3	-17.09	120.75	129.30
22	BA	2051	A	N1-C2-N3	-17.09	120.75	129.30
23	BB	58	A	N1-C2-N3	-17.09	120.76	129.30
1	AA	1271	A	N1-C2-N3	-17.09	120.76	129.30
1	AA	495	A	C2-N3-C4	17.09	119.14	110.60
1	AA	520	A	N1-C2-N3	-17.09	120.76	129.30
22	BA	693	A	N1-C2-N3	-17.09	120.76	129.30
22	BA	1801	A	C2-N3-C4	17.08	119.14	110.60
22	BA	788	A	N1-C2-N3	-17.08	120.76	129.30
22	BA	1134	A	N1-C2-N3	-17.08	120.76	129.30
22	BA	1205	A	N1-C2-N3	-17.08	120.76	129.30
1	AA	663	A	N1-C6-N6	-17.08	108.35	118.60
22	BA	44	A	N1-C2-N3	-17.08	120.76	129.30
22	BA	1027	A	N1-C6-N6	-17.08	108.35	118.60
22	BA	1111	A	N1-C6-N6	-17.08	108.35	118.60
22	BA	1919	A	N1-C6-N6	-17.08	108.35	118.60
1	AA	1274	A	N1-C6-N6	-17.08	108.35	118.60
22	BA	1938	A	C2-N3-C4	17.08	119.14	110.60
22	BA	2757	A	N1-C2-N3	-17.08	120.76	129.30
1	AA	1176	A	N1-C6-N6	-17.07	108.36	118.60
1	AA	270	A	N1-C6-N6	-17.07	108.36	118.60
1	AA	459	A	N1-C6-N6	-17.07	108.36	118.60
1	AA	608	A	N1-C6-N6	-17.07	108.36	118.60
22	BA	299	A	N1-C6-N6	-17.07	108.36	118.60
1	AA	642	A	C2-N3-C4	17.06	119.13	110.60
1	AA	270	A	N1-C2-N3	-17.06	120.77	129.30
1	AA	366	A	N1-C2-N3	-17.06	120.77	129.30
22	BA	144	A	N1-C6-N6	-17.06	108.36	118.60
22	BA	1722	A	N1-C2-N3	-17.06	120.77	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1829	A	N1-C2-N3	-17.06	120.77	129.30
22	BA	2082	A	N1-C6-N6	-17.06	108.37	118.60
22	BA	2352	A	N1-C2-N3	-17.05	120.77	129.30
1	AA	1483	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	190	A	N1-C2-N3	-17.05	120.77	129.30
22	BA	2851	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	2432	A	N1-C6-N6	-17.05	108.37	118.60
1	AA	415	A	N1-C2-N3	-17.05	120.78	129.30
1	AA	520	A	C2-N3-C4	17.05	119.12	110.60
1	AA	246	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	56	A	N1-C2-N3	-17.05	120.78	129.30
22	BA	2766	A	N1-C2-N3	-17.05	120.78	129.30
1	AA	448	A	N1-C2-N3	-17.04	120.78	129.30
1	AA	1357	A	N1-C2-N3	-17.04	120.78	129.30
22	BA	2459	A	N1-C6-N6	-17.04	108.37	118.60
22	BA	609	A	C2-N3-C4	17.04	119.12	110.60
22	BA	909	A	N1-C2-N3	-17.04	120.78	129.30
1	AA	983	A	N1-C2-N3	-17.04	120.78	129.30
22	BA	161	A	C2-N3-C4	17.04	119.12	110.60
22	BA	324	A	C2-N3-C4	17.03	119.12	110.60
22	BA	960	A	N1-C2-N3	-17.03	120.78	129.30
22	BA	1953	A	C2-N3-C4	17.03	119.12	110.60
1	AA	155	A	N1-C6-N6	-17.03	108.38	118.60
22	BA	282	A	N1-C6-N6	-17.03	108.38	118.60
55	B8	38	A	N1-C6-N6	-17.03	108.38	118.60
1	AA	98	A	N1-C2-N3	-17.03	120.79	129.30
22	BA	538	A	C2-N3-C4	17.02	119.11	110.60
22	BA	911	A	C2-N3-C4	17.02	119.11	110.60
22	BA	13	A	N1-C2-N3	-17.02	120.79	129.30
1	AA	487	A	N1-C2-N3	-17.01	120.79	129.30
22	BA	1103	A	N1-C2-N3	-17.01	120.79	129.30
22	BA	1354	A	N1-C6-N6	-17.01	108.39	118.60
22	BA	626	A	N1-C6-N6	-17.01	108.39	118.60
1	AA	1492	A	C2-N3-C4	17.01	119.10	110.60
22	BA	2126	A	N1-C2-N3	-17.01	120.80	129.30
22	BA	2082	A	N1-C2-N3	-17.00	120.80	129.30
1	AA	1191	A	N1-C6-N6	-17.00	108.40	118.60
22	BA	2814	A	N1-C2-N3	-17.00	120.80	129.30
1	AA	790	A	N1-C6-N6	-17.00	108.40	118.60
22	BA	1928	A	C2-N3-C4	17.00	119.10	110.60
22	BA	2425	A	N1-C6-N6	-17.00	108.40	118.60
22	BA	522	A	N1-C6-N6	-17.00	108.40	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2432	A	N1-C2-N3	-17.00	120.80	129.30
1	AA	190	A	C2-N3-C4	16.99	119.10	110.60
1	AA	502	A	N1-C6-N6	-16.99	108.41	118.60
22	BA	2297	A	N1-C2-N3	-16.99	120.80	129.30
23	BB	34	A	N1-C6-N6	-16.99	108.41	118.60
1	AA	729	A	N1-C6-N6	-16.99	108.41	118.60
22	BA	95	A	N1-C6-N6	-16.99	108.41	118.60
22	BA	1084	A	N1-C2-N3	-16.98	120.81	129.30
22	BA	1387	A	N1-C2-N3	-16.98	120.81	129.30
22	BA	761	A	C2-N3-C4	16.98	119.09	110.60
1	AA	1431	A	N1-C6-N6	-16.98	108.41	118.60
1	AA	1507	A	N1-C6-N6	-16.98	108.41	118.60
22	BA	575	A	C2-N3-C4	16.98	119.09	110.60
22	BA	1010	A	N1-C6-N6	-16.97	108.42	118.60
22	BA	633	A	C2-N3-C4	16.97	119.09	110.60
22	BA	1689	A	N1-C6-N6	-16.97	108.42	118.60
1	AA	66	A	N1-C6-N6	-16.97	108.42	118.60
22	BA	722	A	N1-C6-N6	-16.97	108.42	118.60
22	BA	176	A	N1-C6-N6	-16.96	108.42	118.60
22	BA	384	A	N1-C2-N3	-16.96	120.82	129.30
22	BA	1552	A	C2-N3-C4	16.96	119.08	110.60
22	BA	1876	A	N1-C6-N6	-16.96	108.42	118.60
22	BA	1134	A	C2-N3-C4	16.96	119.08	110.60
22	BA	2013	A	C2-N3-C4	16.96	119.08	110.60
22	BA	590	A	N1-C2-N3	-16.96	120.82	129.30
1	AA	649	A	N1-C2-N3	-16.95	120.82	129.30
1	AA	630	A	N1-C6-N6	-16.95	108.43	118.60
1	AA	33	A	N1-C6-N6	-16.95	108.43	118.60
1	AA	1274	A	C2-N3-C4	16.95	119.08	110.60
1	AA	1418	A	N1-C2-N3	-16.95	120.82	129.30
22	BA	1133	A	N1-C2-N3	-16.95	120.83	129.30
22	BA	1393	A	C2-N3-C4	16.95	119.08	110.60
22	BA	1572	A	N1-C2-N3	-16.95	120.83	129.30
1	AA	338	A	N1-C2-N3	-16.95	120.83	129.30
1	AA	279	A	C2-N3-C4	16.95	119.07	110.60
1	AA	865	A	N1-C2-N3	-16.95	120.83	129.30
22	BA	1637	A	N1-C2-N3	-16.95	120.83	129.30
22	BA	1641	A	N1-C2-N3	-16.95	120.83	129.30
22	BA	1654	A	N1-C6-N6	-16.95	108.43	118.60
1	AA	1508	A	N1-C6-N6	-16.94	108.43	118.60
1	AA	743	A	N1-C6-N6	-16.94	108.44	118.60
22	BA	1276	A	N1-C6-N6	-16.94	108.44	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1545	A	N1-C2-N3	-16.94	120.83	129.30
22	BA	152	A	C2-N3-C4	16.93	119.07	110.60
22	BA	1098	A	N1-C6-N6	-16.93	108.44	118.60
1	AA	663	A	N1-C2-N3	-16.93	120.84	129.30
1	AA	864	A	N1-C2-N3	-16.92	120.84	129.30
1	AA	1465	A	N1-C2-N3	-16.92	120.84	129.30
22	BA	1701	A	C2-N3-C4	16.92	119.06	110.60
22	BA	1829	A	N1-C6-N6	-16.92	108.45	118.60
1	AA	681	A	N1-C6-N6	-16.92	108.45	118.60
22	BA	2516	A	N1-C2-N3	-16.92	120.84	129.30
1	AA	338	A	N1-C6-N6	-16.91	108.45	118.60
1	AA	498	A	N1-C6-N6	-16.91	108.45	118.60
1	AA	782	A	N1-C2-N3	-16.91	120.84	129.30
22	BA	480	A	N1-C6-N6	-16.91	108.45	118.60
22	BA	788	A	C2-N3-C4	16.91	119.05	110.60
22	BA	2761	A	N1-C2-N3	-16.91	120.84	129.30
1	AA	228	A	N1-C6-N6	-16.90	108.46	118.60
1	AA	1102	A	N1-C2-N3	-16.90	120.85	129.30
22	BA	505	A	N1-C2-N3	-16.90	120.85	129.30
22	BA	6	A	C2-N3-C4	16.89	119.05	110.60
22	BA	255	A	N1-C6-N6	-16.89	108.47	118.60
22	BA	2059	A	N1-C2-N3	-16.89	120.86	129.30
22	BA	2741	A	N1-C2-N3	-16.89	120.86	129.30
22	BA	1469	A	N1-C6-N6	-16.89	108.47	118.60
1	AA	1204	A	C2-N3-C4	16.88	119.04	110.60
22	BA	2435	A	N1-C6-N6	-16.88	108.47	118.60
22	BA	632	A	N1-C6-N6	-16.87	108.48	118.60
1	AA	356	A	N1-C6-N6	-16.87	108.48	118.60
22	BA	735	A	N1-C6-N6	-16.86	108.48	118.60
22	BA	1552	A	N1-C6-N6	-16.86	108.48	118.60
22	BA	2497	A	N1-C2-N3	-16.86	120.87	129.30
22	BA	1275	A	C2-N3-C4	16.85	119.03	110.60
22	BA	1285	A	N1-C2-N3	-16.85	120.87	129.30
22	BA	52	A	N1-C6-N6	-16.85	108.49	118.60
22	BA	849	A	C2-N3-C4	16.85	119.02	110.60
1	AA	74	A	C2-N3-C4	16.84	119.02	110.60
22	BA	1679	A	N1-C2-N3	-16.84	120.88	129.30
1	AA	642	A	N1-C2-N3	-16.84	120.88	129.30
22	BA	2015	A	N1-C6-N6	-16.84	108.50	118.60
22	BA	354	A	N1-C2-N3	-16.84	120.88	129.30
22	BA	730	A	N1-C2-N3	-16.84	120.88	129.30
22	BA	1938	A	N1-C6-N6	-16.84	108.50	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	559	A	C2-N3-C4	16.83	119.02	110.60
1	AA	768	A	N1-C2-N3	-16.83	120.89	129.30
1	AA	1408	A	C2-N3-C4	16.83	119.01	110.60
1	AA	373	A	N1-C2-N3	-16.82	120.89	129.30
22	BA	1133	A	N1-C6-N6	-16.82	108.51	118.60
22	BA	2059	A	C2-N3-C4	16.82	119.01	110.60
22	BA	2706	A	N1-C2-N3	-16.82	120.89	129.30
22	BA	182	A	N1-C2-N3	-16.82	120.89	129.30
22	BA	2142	A	N1-C2-N3	-16.81	120.89	129.30
22	BA	1413	A	N1-C6-N6	-16.80	108.52	118.60
1	AA	452	A	N1-C6-N6	-16.80	108.52	118.60
22	BA	404	A	C2-N3-C4	16.80	119.00	110.60
22	BA	2600	A	C2-N3-C4	16.80	119.00	110.60
1	AA	729	A	N1-C2-N3	-16.79	120.90	129.30
1	AA	782	A	C2-N3-C4	16.79	119.00	110.60
22	BA	1773	A	C2-N3-C4	16.79	119.00	110.60
22	BA	1241	A	N1-C2-N3	-16.79	120.91	129.30
22	BA	1616	A	C2-N3-C4	16.79	118.99	110.60
22	BA	2088	A	N1-C6-N6	-16.79	108.53	118.60
22	BA	197	A	C2-N3-C4	16.78	118.99	110.60
22	BA	1614	A	N1-C2-N3	-16.78	120.91	129.30
1	AA	1493	A	C2-N3-C4	16.78	118.99	110.60
22	BA	233	A	N1-C6-N6	-16.77	108.54	118.60
22	BA	6	A	N1-C6-N6	-16.77	108.54	118.60
22	BA	352	A	N1-C6-N6	-16.77	108.54	118.60
1	AA	563	A	N1-C2-N3	-16.76	120.92	129.30
22	BA	2013	A	N1-C2-N3	-16.76	120.92	129.30
22	BA	2679	A	N1-C6-N6	-16.76	108.54	118.60
1	AA	19	A	N1-C2-N3	-16.76	120.92	129.30
22	BA	2020	A	N1-C2-N3	-16.76	120.92	129.30
1	AA	790	A	N1-C2-N3	-16.75	120.92	129.30
22	BA	1652	A	N1-C2-N3	-16.75	120.92	129.30
22	BA	2378	A	N1-C6-N6	-16.75	108.55	118.60
22	BA	2721	A	C2-N3-C4	16.75	118.98	110.60
1	AA	1375	A	N1-C6-N6	-16.74	108.56	118.60
22	BA	677	A	N1-C6-N6	-16.74	108.56	118.60
1	AA	1170	A	C2-N3-C4	16.72	118.96	110.60
22	BA	572	A	N1-C6-N6	-16.72	108.57	118.60
22	BA	477	A	N1-C2-N3	-16.71	120.94	129.30
22	BA	2461	A	N1-C6-N6	-16.71	108.57	118.60
22	BA	2534	A	N1-C2-N3	-16.71	120.94	129.30
1	AA	55	A	N1-C6-N6	-16.70	108.58	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1614	A	C2-N3-C4	16.69	118.95	110.60
22	BA	752	A	N1-C2-N3	-16.69	120.95	129.30
1	AA	1216	A	N1-C2-N3	-16.69	120.96	129.30
1	AA	767	A	N1-C6-N6	-16.68	108.59	118.60
22	BA	505	A	N1-C6-N6	-16.68	108.59	118.60
1	AA	1227	A	C2-N3-C4	16.68	118.94	110.60
22	BA	311	A	C2-N3-C4	16.67	118.94	110.60
1	AA	397	A	N1-C2-N3	-16.66	120.97	129.30
22	BA	705	A	N1-C6-N6	-16.66	108.60	118.60
22	BA	2097	A	N1-C6-N6	-16.66	108.60	118.60
1	AA	559	A	N1-C2-N3	-16.66	120.97	129.30
22	BA	2900	A	N1-C2-N3	-16.65	120.97	129.30
1	AA	502	A	N1-C2-N3	-16.64	120.98	129.30
22	BA	1919	A	C2-N3-C4	16.64	118.92	110.60
23	BB	66	A	N1-C2-N3	-16.64	120.98	129.30
22	BA	1678	A	C2-N3-C4	16.63	118.92	110.60
22	BA	1872	A	C2-N3-C4	16.63	118.92	110.60
22	BA	1413	A	N1-C2-N3	-16.63	120.98	129.30
22	BA	2721	A	N1-C2-N3	-16.63	120.98	129.30
22	BA	863	A	N1-C2-N3	-16.63	120.99	129.30
22	BA	1021	A	N1-C2-N3	-16.63	120.99	129.30
22	BA	477	A	N1-C6-N6	-16.62	108.63	118.60
22	BA	2077	A	N1-C2-N3	-16.62	120.99	129.30
22	BA	2108	A	C2-N3-C4	16.62	118.91	110.60
22	BA	1133	A	C2-N3-C4	16.61	118.91	110.60
22	BA	861	A	N1-C6-N6	-16.61	108.63	118.60
22	BA	666	A	N1-C6-N6	-16.61	108.64	118.60
22	BA	2727	A	N1-C6-N6	-16.60	108.64	118.60
22	BA	1244	A	N1-C6-N6	-16.60	108.64	118.60
22	BA	781	A	N1-C2-N3	-16.60	121.00	129.30
1	AA	706	A	N1-C6-N6	-16.60	108.64	118.60
22	BA	2407	A	N1-C2-N3	-16.60	121.00	129.30
22	BA	149	A	N1-C2-N3	-16.60	121.00	129.30
22	BA	756	A	N1-C6-N6	-16.59	108.64	118.60
22	BA	833	A	N1-C2-N3	-16.59	121.00	129.30
22	BA	311	A	N1-C6-N6	-16.59	108.65	118.60
1	AA	1375	A	C2-N3-C4	16.59	118.89	110.60
1	AA	300	A	C2-N3-C4	16.58	118.89	110.60
22	BA	1226	A	C2-N3-C4	16.58	118.89	110.60
22	BA	2369	A	N1-C6-N6	-16.58	108.65	118.60
1	AA	32	A	N1-C2-N3	-16.57	121.01	129.30
22	BA	503	A	N1-C2-N3	-16.57	121.02	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1431	A	N1-C2-N3	-16.57	121.02	129.30
22	BA	2814	A	C2-N3-C4	16.57	118.88	110.60
22	BA	384	A	C2-N3-C4	16.56	118.88	110.60
22	BA	324	A	N1-C6-N6	-16.55	108.67	118.60
22	BA	1722	A	N1-C6-N6	-16.55	108.67	118.60
22	BA	2670	A	N1-C2-N3	-16.54	121.03	129.30
1	AA	1433	A	C2-N3-C4	16.54	118.87	110.60
22	BA	1757	A	C2-N3-C4	16.53	118.87	110.60
1	AA	1339	A	N1-C2-N3	-16.53	121.04	129.30
22	BA	2757	A	N1-C6-N6	-16.53	108.68	118.60
22	BA	126	A	N1-C6-N6	-16.52	108.69	118.60
1	AA	325	A	C2-N3-C4	16.51	118.86	110.60
1	AA	865	A	N1-C6-N6	-16.51	108.69	118.60
22	BA	644	A	N1-C2-N3	-16.51	121.04	129.30
22	BA	2461	A	N1-C2-N3	-16.51	121.05	129.30
22	BA	449	A	N1-C2-N3	-16.50	121.05	129.30
1	AA	66	A	C2-N3-C4	16.50	118.85	110.60
22	BA	2071	A	N1-C2-N3	-16.50	121.05	129.30
22	BA	582	A	N1-C6-N6	-16.50	108.70	118.60
1	AA	199	A	N1-C2-N3	-16.49	121.06	129.30
1	AA	1171	A	N1-C2-N3	-16.48	121.06	129.30
22	BA	2418	A	N1-C6-N6	-16.47	108.72	118.60
1	AA	746	A	N1-C2-N3	-16.47	121.07	129.30
1	AA	325	A	N1-C2-N3	-16.46	121.07	129.30
22	BA	422	A	N1-C2-N3	-16.45	121.08	129.30
22	BA	63	A	N1-C6-N6	-16.45	108.73	118.60
22	BA	1810	A	N1-C2-N3	-16.44	121.08	129.30
23	BB	39	A	N1-C6-N6	-16.44	108.74	118.60
1	AA	1357	A	N1-C6-N6	-16.44	108.74	118.60
1	AA	1508	A	N1-C2-N3	-16.44	121.08	129.30
1	AA	743	A	N1-C2-N3	-16.43	121.08	129.30
22	BA	975	A	N1-C2-N3	-16.42	121.09	129.30
22	BA	2108	A	N1-C6-N6	-16.42	108.75	118.60
22	BA	2530	A	N1-C2-N3	-16.42	121.09	129.30
1	AA	223	A	N1-C2-N3	-16.41	121.09	129.30
1	AA	77	A	N1-C2-N3	-16.41	121.09	129.30
1	AA	1299	A	N1-C2-N3	-16.41	121.09	129.30
22	BA	1668	A	C2-N3-C4	16.41	118.80	110.60
22	BA	453	A	N1-C6-N6	-16.40	108.76	118.60
22	BA	1609	A	N1-C6-N6	-16.39	108.77	118.60
1	AA	978	A	N1-C2-N3	-16.39	121.11	129.30
22	BA	2108	A	N1-C2-N3	-16.39	121.11	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	397	A	N1-C6-N6	-16.38	108.77	118.60
1	AA	162	A	N1-C2-N3	-16.38	121.11	129.30
23	BB	59	A	N1-C6-N6	-16.38	108.77	118.60
22	BA	1155	A	N1-C6-N6	-16.38	108.77	118.60
22	BA	1143	A	N1-C6-N6	-16.38	108.78	118.60
22	BA	2284	A	N1-C2-N3	-16.38	121.11	129.30
22	BA	2531	A	N1-C2-N3	-16.37	121.11	129.30
22	BA	1213	A	N1-C6-N6	-16.37	108.78	118.60
22	BA	2095	A	N1-C2-N3	-16.36	121.12	129.30
22	BA	1866	A	N1-C6-N6	-16.35	108.79	118.60
22	BA	472	A	N1-C6-N6	-16.35	108.79	118.60
1	AA	1375	A	N1-C2-N3	-16.35	121.13	129.30
22	BA	1571	A	N1-C6-N6	-16.35	108.79	118.60
22	BA	2090	A	N1-C6-N6	-16.34	108.80	118.60
22	BA	2430	A	N1-C2-N3	-16.34	121.13	129.30
23	BB	66	A	C2-N3-C4	16.34	118.77	110.60
22	BA	751	A	N1-C6-N6	-16.34	108.80	118.60
1	AA	706	A	N1-C2-N3	-16.32	121.14	129.30
22	BA	1664	A	N1-C2-N3	-16.30	121.15	129.30
22	BA	936	A	N1-C6-N6	-16.29	108.82	118.60
22	BA	352	A	N1-C2-N3	-16.27	121.16	129.30
22	BA	2670	A	N1-C6-N6	-16.27	108.84	118.60
22	BA	2662	A	N1-C6-N6	-16.26	108.84	118.60
22	BA	101	A	N1-C2-N3	-16.25	121.17	129.30
1	AA	55	A	N1-C2-N3	-16.25	121.17	129.30
1	AA	1219	A	N1-C6-N6	-16.25	108.85	118.60
22	BA	362	A	N1-C6-N6	-16.25	108.85	118.60
22	BA	742	A	N1-C6-N6	-16.25	108.85	118.60
1	AA	77	A	N1-C6-N6	-16.24	108.86	118.60
22	BA	2675	A	N1-C6-N6	-16.24	108.86	118.60
1	AA	181	A	N1-C6-N6	-16.24	108.86	118.60
1	AA	718	A	N1-C6-N6	-16.23	108.86	118.60
22	BA	1978	A	N1-C6-N6	-16.23	108.86	118.60
22	BA	1773	A	N1-C2-N3	-16.22	121.19	129.30
22	BA	1678	A	N1-C2-N3	-16.21	121.19	129.30
55	B8	66	A	N1-C6-N6	-16.21	108.87	118.60
22	BA	2297	A	C2-N3-C4	16.20	118.70	110.60
22	BA	2077	A	N1-C6-N6	-16.20	108.88	118.60
22	BA	1705	A	N1-C6-N6	-16.20	108.88	118.60
1	AA	300	A	N1-C2-N3	-16.19	121.21	129.30
1	AA	1170	A	N1-C2-N3	-16.19	121.21	129.30
22	BA	2013	A	N1-C6-N6	-16.18	108.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	983	A	C2-N3-C4	16.18	118.69	110.60
22	BA	599	A	N1-C6-N6	-16.16	108.90	118.60
22	BA	223	A	N1-C6-N6	-16.15	108.91	118.60
22	BA	705	A	N1-C2-N3	-16.14	121.23	129.30
22	BA	2241	A	N1-C6-N6	-16.13	108.92	118.60
22	BA	391	A	N1-C6-N6	-16.13	108.92	118.60
22	BA	1134	A	N1-C6-N6	-16.13	108.92	118.60
22	BA	2577	A	N1-C2-N3	-16.13	121.24	129.30
22	BA	2893	A	N1-C6-N6	-16.12	108.92	118.60
1	AA	383	A	C2-N3-C4	16.12	118.66	110.60
1	AA	696	A	N1-C6-N6	-16.11	108.94	118.60
1	AA	1055	A	N1-C6-N6	-16.09	108.94	118.60
1	AA	32	A	N1-C6-N6	-16.09	108.95	118.60
1	AA	66	A	N1-C2-N3	-16.08	121.26	129.30
1	AA	554	A	N1-C2-N3	-16.07	121.27	129.30
22	BA	1872	A	N1-C2-N3	-16.07	121.27	129.30
22	BA	2287	A	N1-C6-N6	-16.07	108.96	118.60
1	AA	784	A	N1-C2-N3	-16.06	121.27	129.30
22	BA	575	A	N1-C6-N6	-16.06	108.97	118.60
22	BA	2386	A	N1-C6-N6	-16.04	108.98	118.60
22	BA	231	A	N1-C2-N3	-16.03	121.28	129.30
1	AA	74	A	N1-C2-N3	-16.03	121.29	129.30
22	BA	2225	A	C2-N3-C4	16.02	118.61	110.60
22	BA	2433	A	N1-C6-N6	-16.02	108.99	118.60
1	AA	1197	A	N1-C6-N6	-16.01	109.00	118.60
22	BA	1677	A	N1-C2-N3	-16.01	121.30	129.30
1	AA	978	A	C2-N3-C4	16.00	118.60	110.60
22	BA	2725	A	N1-C6-N6	-16.00	109.00	118.60
1	AA	923	A	N1-C6-N6	-15.99	109.00	118.60
22	BA	1021	A	N1-C6-N6	-15.99	109.01	118.60
22	BA	2225	A	N1-C6-N6	-15.99	109.01	118.60
1	AA	1339	A	N1-C6-N6	-15.94	109.03	118.60
22	BA	2482	A	N1-C6-N6	-15.94	109.03	118.60
22	BA	1626	A	N1-C6-N6	-15.94	109.04	118.60
22	BA	197	A	N1-C6-N6	-15.94	109.04	118.60
22	BA	131	A	N1-C2-N3	-15.92	121.34	129.30
1	AA	1360	A	N1-C2-N3	-15.91	121.34	129.30
22	BA	415	A	N1-C6-N6	-15.91	109.06	118.60
22	BA	833	A	N1-C6-N6	-15.90	109.06	118.60
1	AA	923	A	N1-C2-N3	-15.90	121.35	129.30
1	AA	28	A	N1-C6-N6	-15.89	109.07	118.60
22	BA	2600	A	N1-C2-N3	-15.88	121.36	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1373	A	N1-C6-N6	-15.88	109.07	118.60
1	AA	901	A	N1-C2-N3	-15.87	121.36	129.30
22	BA	19	A	N1-C6-N6	-15.86	109.08	118.60
1	AA	411	A	N1-C6-N6	-15.86	109.08	118.60
22	BA	1977	A	N1-C6-N6	-15.86	109.08	118.60
22	BA	2820	A	C2-N3-C4	15.85	118.53	110.60
22	BA	352	A	C2-N3-C4	15.82	118.51	110.60
22	BA	1387	A	N1-C6-N6	-15.82	109.11	118.60
22	BA	947	A	N1-C6-N6	-15.81	109.11	118.60
1	AA	190	A	N1-C2-N3	-15.81	121.40	129.30
1	AA	1339	A	C2-N3-C4	15.80	118.50	110.60
22	BA	996	A	N1-C6-N6	-15.79	109.13	118.60
22	BA	1872	A	N1-C6-N6	-15.78	109.13	118.60
22	BA	1553	A	N1-C6-N6	-15.74	109.16	118.60
1	AA	673	A	N1-C2-N3	-15.73	121.43	129.30
22	BA	482	A	N1-C2-N3	-15.71	121.45	129.30
22	BA	1970	A	O5'-P-OP1	-15.70	91.57	105.70
22	BA	1669	A	N1-C2-N3	-15.64	121.48	129.30
1	AA	371	A	N1-C2-N3	-15.64	121.48	129.30
22	BA	1854	A	N1-C6-N6	-15.63	109.22	118.60
22	BA	251	A	C2-N3-C4	15.60	118.40	110.60
1	AA	1319	A	C2-N3-C4	15.60	118.40	110.60
22	BA	1669	A	N1-C6-N6	-15.59	109.25	118.60
22	BA	2813	A	N1-C6-N6	-15.58	109.25	118.60
22	BA	849	A	N1-C2-N3	-15.57	121.51	129.30
1	AA	860	A	N1-C2-N3	-15.56	121.52	129.30
55	B8	19	G	OP1-P-O3'	-15.56	70.96	105.20
22	BA	2333	A	N1-C6-N6	-15.54	109.27	118.60
22	BA	470	A	N1-C6-N6	-15.50	109.30	118.60
1	AA	533	A	N1-C2-N3	-15.49	121.55	129.30
22	BA	761	A	N1-C2-N3	-15.49	121.56	129.30
1	AA	1046	A	N1-C2-N3	-15.48	121.56	129.30
1	AA	1201	A	N1-C6-N6	-15.48	109.31	118.60
22	BA	1269	A	N1-C2-N3	-15.47	121.56	129.30
1	AA	1468	A	N1-C6-N6	-15.46	109.32	118.60
22	BA	1641	A	N1-C6-N6	-15.45	109.33	118.60
22	BA	430	A	N1-C6-N6	-15.45	109.33	118.60
22	BA	2042	A	N1-C6-N6	-15.45	109.33	118.60
22	BA	845	A	N1-C6-N6	-15.44	109.33	118.60
22	BA	2614	A	N1-C2-N3	-15.44	121.58	129.30
1	AA	383	A	N1-C2-N3	-15.40	121.60	129.30
22	BA	849	A	N1-C6-N6	-15.38	109.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1246	A	N1-C2-N3	-15.38	121.61	129.30
22	BA	2430	A	C5-C6-N6	15.36	135.99	123.70
22	BA	1528	A	N1-C6-N6	-15.36	109.39	118.60
1	AA	1201	A	N1-C2-N3	-15.35	121.63	129.30
22	BA	631	A	N1-C6-N6	-15.35	109.39	118.60
1	AA	431	A	C5-C6-N6	15.34	135.97	123.70
22	BA	2020	A	N1-C6-N6	-15.34	109.40	118.60
1	AA	563	A	N1-C6-N6	-15.30	109.42	118.60
1	AA	452	A	N1-C2-N3	-15.27	121.67	129.30
22	BA	983	A	N1-C6-N6	-15.25	109.45	118.60
22	BA	1434	A	C5-C6-N6	15.21	135.87	123.70
1	AA	1418	A	N1-C6-N6	-15.21	109.47	118.60
22	BA	101	A	N1-C6-N6	-15.20	109.48	118.60
22	BA	131	A	N1-C6-N6	-15.13	109.52	118.60
22	BA	1677	A	C2-N3-C4	15.13	118.16	110.60
22	BA	863	A	N1-C6-N6	-15.11	109.53	118.60
22	BA	793	A	N1-C6-N6	-15.09	109.54	118.60
22	BA	513	A	N1-C6-N6	-15.02	109.59	118.60
1	AA	465	A	N7-C8-N9	-14.96	106.32	113.80
22	BA	482	A	N1-C6-N6	-14.95	109.63	118.60
22	BA	1664	A	N1-C6-N6	-14.95	109.63	118.60
22	BA	152	A	N1-C6-N6	-14.92	109.65	118.60
22	BA	2407	A	N1-C6-N6	-14.84	109.69	118.60
1	AA	1204	A	N1-C2-N3	-14.80	121.90	129.30
22	BA	1668	A	C5-C6-N6	14.64	135.41	123.70
1	AA	901	A	N1-C6-N6	-14.63	109.82	118.60
22	BA	251	A	N1-C6-N6	-14.62	109.83	118.60
1	AA	162	A	N1-C6-N6	-14.59	109.84	118.60
22	BA	251	A	N1-C2-N3	-14.59	122.00	129.30
2	AB	205	ASP	CB-CG-OD1	14.46	131.32	118.30
22	BA	586	A	C5-C6-N6	14.43	135.25	123.70
2	AB	204	ASP	N-CA-CB	-14.40	84.67	110.60
23	BB	101	A	N3-C4-C5	-14.40	116.72	126.80
22	BA	1970	A	C2-N3-C4	14.40	117.80	110.60
22	BA	2600	A	N1-C6-N6	-14.34	110.00	118.60
22	BA	2799	A	N1-C6-N6	-14.31	110.02	118.60
22	BA	960	A	N1-C6-N6	-14.26	110.04	118.60
22	BA	792	A	N1-C6-N6	-14.22	110.06	118.60
1	AA	1170	A	N1-C6-N6	-14.22	110.07	118.60
22	BA	1241	A	N1-C6-N6	-14.18	110.09	118.60
1	AA	1213	A	C5-C6-N6	14.02	134.91	123.70
22	BA	800	A	C5-C6-N6	13.95	134.86	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	699	A	C5-C6-N6	13.93	134.85	123.70
22	BA	1285	A	C5-C6-N6	13.87	134.79	123.70
22	BA	457	A	C5-C6-N6	13.85	134.78	123.70
22	BA	804	A	C5-C6-N6	13.75	134.70	123.70
22	BA	1937	A	C5-C6-N6	13.73	134.69	123.70
1	AA	498	A	N1-C2-N3	-13.71	122.44	129.30
22	BA	1810	A	N1-C6-N6	-13.70	110.38	118.60
22	BA	781	A	C5-C6-N6	13.67	134.64	123.70
22	BA	1970	A	N1-C6-N6	-13.66	110.41	118.60
1	AA	1446	A	C5-C6-N6	13.64	134.62	123.70
22	BA	941	A	C5-C6-N6	13.64	134.62	123.70
22	BA	515	A	C5-C6-N6	13.64	134.61	123.70
22	BA	1677	A	N1-C6-N6	-13.64	110.42	118.60
22	BA	911	A	N1-C6-N6	-13.59	110.44	118.60
22	BA	2726	A	C5-C6-N6	13.59	134.57	123.70
23	BB	59	A	N1-C2-N3	-13.59	122.50	129.30
22	BA	479	A	C5-C6-N6	13.57	134.56	123.70
22	BA	764	A	C5-C6-N6	13.56	134.55	123.70
22	BA	13	A	C5-C6-N6	13.54	134.54	123.70
22	BA	1253	A	C5-C6-N6	13.49	134.49	123.70
22	BA	502	A	C5-C6-N6	13.48	134.49	123.70
23	BB	59	A	N3-C4-C5	-13.47	117.37	126.80
22	BA	1275	A	C5-C6-N6	13.45	134.46	123.70
22	BA	2764	A	C5-C6-N6	13.40	134.42	123.70
1	AA	520	A	C5-C6-N6	13.33	134.36	123.70
22	BA	2882	A	C5-C6-N6	13.32	134.36	123.70
22	BA	2450	A	C5-C6-N6	13.30	134.34	123.70
22	BA	563	A	C5-C6-N6	13.29	134.34	123.70
22	BA	621	A	C5-C6-N6	13.29	134.34	123.70
55	B8	6	A	N7-C8-N9	-13.28	107.16	113.80
1	AA	300	A	N1-C6-N6	-13.27	110.64	118.60
22	BA	2598	A	C5-C6-N6	13.27	134.32	123.70
1	AA	1332	A	N7-C8-N9	-13.26	107.17	113.80
22	BA	783	A	C5-C6-N6	13.26	134.31	123.70
1	AA	1319	A	N7-C8-N9	-13.23	107.19	113.80
22	BA	1789	A	C5-C6-N6	13.23	134.28	123.70
22	BA	975	A	C5-C6-N6	13.19	134.25	123.70
1	AA	498	A	N3-C4-C5	-13.17	117.58	126.80
22	BA	119	A	C5-C6-N6	13.17	134.23	123.70
22	BA	2033	A	C5-C6-N6	13.15	134.22	123.70
22	BA	2872	A	N9-C4-C5	13.14	111.06	105.80
1	AA	274	A	N7-C8-N9	-13.14	107.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	207	A	C5-C6-N6	13.13	134.20	123.70
22	BA	165	A	C5-C6-N6	13.12	134.20	123.70
22	BA	241	A	C5-C6-N6	13.11	134.18	123.70
22	BA	529	A	C5-C6-N6	13.11	134.19	123.70
22	BA	2577	A	C5-C6-N6	13.10	134.18	123.70
22	BA	466	A	C5-C6-N6	13.10	134.18	123.70
22	BA	752	A	C5-C6-N6	13.10	134.18	123.70
22	BA	141	G	C5-N7-C8	-13.05	97.77	104.30
1	AA	1299	A	C5-C6-N6	13.04	134.14	123.70
22	BA	1214	A	C5-C6-N6	13.03	134.12	123.70
22	BA	2448	A	C5-C6-N6	13.03	134.13	123.70
22	BA	322	A	C5-C6-N6	13.02	134.12	123.70
55	B8	58	A	N7-C8-N9	-13.02	107.29	113.80
22	BA	2826	A	C5-C6-N6	13.01	134.11	123.70
22	BA	1821	A	C5-C6-N6	13.00	134.10	123.70
22	BA	761	A	C5-C6-N6	12.99	134.09	123.70
1	AA	889	A	C5-C6-N6	12.98	134.08	123.70
22	BA	2758	A	C5-C6-N6	12.97	134.08	123.70
22	BA	2590	A	C5-C6-N6	12.95	134.06	123.70
22	BA	2753	A	C5-C6-N6	12.91	134.03	123.70
22	BA	2572	A	N7-C8-N9	-12.90	107.35	113.80
22	BA	2721	A	C5-C6-N6	12.87	134.00	123.70
22	BA	675	A	C5-C6-N6	12.82	133.95	123.70
22	BA	2823	A	C5-C6-N6	12.82	133.95	123.70
22	BA	2060	A	C5-C6-N6	12.81	133.95	123.70
23	BB	46	A	C5-C6-N6	12.80	133.94	123.70
22	BA	1308	A	C5-C6-N6	12.79	133.93	123.70
1	AA	777	A	C5-C6-N6	12.77	133.91	123.70
22	BA	1853	A	C5-C6-N6	12.76	133.90	123.70
22	BA	734	A	C5-C6-N6	12.74	133.89	123.70
22	BA	1890	A	C5-C6-N6	12.74	133.89	123.70
1	AA	819	A	C5-C6-N6	12.73	133.88	123.70
22	BA	2005	A	C5-C6-N6	12.73	133.88	123.70
22	BA	217	A	C5-C6-N6	12.72	133.88	123.70
22	BA	1000	A	C5-C6-N6	12.71	133.87	123.70
1	AA	1332	A	C5-C6-N6	12.69	133.85	123.70
22	BA	1754	A	C5-C6-N6	12.69	133.85	123.70
22	BA	1545	A	C5-C6-N6	12.68	133.84	123.70
1	AA	190	A	N1-C6-N6	-12.66	111.00	118.60
22	BA	1205	A	C5-C6-N6	12.66	133.83	123.70
22	BA	1819	A	C5-C6-N6	12.66	133.82	123.70
22	BA	2572	A	C5-C6-N6	12.64	133.81	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1889	A	C5-C6-N6	12.63	133.81	123.70
22	BA	1848	A	C5-C6-N6	12.63	133.80	123.70
22	BA	514	A	C5-C6-N6	12.63	133.80	123.70
22	BA	478	A	C5-C6-N6	12.62	133.79	123.70
22	BA	730	A	N1-C6-N6	-12.62	111.03	118.60
22	BA	984	A	C5-C6-N6	12.62	133.80	123.70
1	AA	665	A	C5-C6-N6	12.61	133.79	123.70
22	BA	1395	A	C5-C6-N6	12.61	133.79	123.70
55	B8	51	A	N7-C8-N9	-12.59	107.51	113.80
1	AA	1502	A	C5-C6-N6	12.58	133.76	123.70
22	BA	782	A	C5-C6-N6	12.57	133.76	123.70
22	BA	1551	A	C5-C6-N6	12.57	133.76	123.70
22	BA	2810	A	C5-C6-N6	12.53	133.72	123.70
1	AA	16	A	C5-C6-N6	12.52	133.72	123.70
22	BA	2749	A	C5-C6-N6	12.52	133.71	123.70
22	BA	979	A	C5-C6-N6	12.51	133.70	123.70
1	AA	704	A	C5-C6-N6	12.50	133.70	123.70
22	BA	216	A	C5-C6-N6	12.49	133.70	123.70
1	AA	607	A	C5-C6-N6	12.49	133.69	123.70
22	BA	2589	A	C5-C6-N6	12.48	133.68	123.70
22	BA	2873	A	C5-C6-N6	12.48	133.68	123.70
22	BA	990	A	C5-C6-N6	12.48	133.68	123.70
22	BA	2014	A	C5-C6-N6	12.48	133.68	123.70
22	BA	1787	A	N3-C4-C5	-12.46	118.07	126.80
1	AA	1340	A	N7-C8-N9	-12.46	107.57	113.80
22	BA	1630	A	C5-C6-N6	12.46	133.66	123.70
22	BA	2741	A	C5-C6-N6	12.45	133.66	123.70
22	BA	1544	A	C5-C6-N6	12.45	133.66	123.70
22	BA	2358	A	C5-C6-N6	12.45	133.66	123.70
2	AB	204	ASP	CB-CG-OD2	-12.44	107.11	118.30
22	BA	1786	A	C5-C6-N6	12.44	133.65	123.70
22	BA	1265	A	C5-C6-N6	12.43	133.65	123.70
22	BA	1791	A	C5-C6-N6	12.42	133.63	123.70
22	BA	2274	A	C5-C6-N6	12.42	133.63	123.70
1	AA	860	A	C5-C6-N6	12.41	133.63	123.70
22	BA	2406	A	C5-C6-N6	12.41	133.63	123.70
22	BA	84	A	C5-C6-N6	12.41	133.63	123.70
1	AA	802	A	C5-C6-N6	12.41	133.63	123.70
22	BA	973	A	C5-C6-N6	12.40	133.62	123.70
1	AA	321	A	C5-C6-N6	12.40	133.62	123.70
22	BA	2835	A	C5-C6-N6	12.38	133.61	123.70
1	AA	1239	A	C5-C6-N6	12.37	133.60	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	310	A	C5-C6-N6	12.36	133.59	123.70
22	BA	1286	A	C5-C6-N6	12.36	133.59	123.70
1	AA	958	A	C5-C6-N6	12.35	133.58	123.70
22	BA	203	A	C5-C6-N6	12.35	133.58	123.70
22	BA	2883	A	C5-C6-N6	12.35	133.58	123.70
1	AA	978	A	C5-C6-N6	12.33	133.56	123.70
1	AA	383	A	N1-C6-N6	-12.32	111.21	118.60
22	BA	504	A	N7-C8-N9	-12.32	107.64	113.80
22	BA	160	A	C5-C6-N6	12.30	133.54	123.70
22	BA	959	A	N7-C8-N9	-12.28	107.66	113.80
22	BA	927	A	C5-C6-N6	12.28	133.53	123.70
22	BA	1970	A	N7-C8-N9	-12.28	107.66	113.80
22	BA	2776	A	C5-C6-N6	12.28	133.53	123.70
22	BA	1366	A	C5-C6-N6	12.28	133.53	123.70
1	AA	919	A	C5-C6-N6	12.27	133.52	123.70
22	BA	2860	A	C5-C6-N6	12.27	133.51	123.70
22	BA	1420	A	C5-C6-N6	12.27	133.51	123.70
22	BA	2614	A	N3-C4-C5	-12.27	118.21	126.80
1	AA	792	A	N7-C8-N9	-12.26	107.67	113.80
55	B8	41	A	N7-C8-N9	-12.26	107.67	113.80
22	BA	1204	A	C5-C6-N6	12.24	133.49	123.70
55	B8	20	U	C5-C6-N1	-12.24	116.58	122.70
1	AA	120	A	C5-C6-N6	12.23	133.49	123.70
22	BA	1569	A	C5-C6-N6	12.23	133.49	123.70
22	BA	1981	A	C5-C6-N6	12.23	133.49	123.70
1	AA	996	A	C5-C6-N6	12.22	133.48	123.70
22	BA	918	A	C5-C6-N6	12.22	133.48	123.70
22	BA	190	A	C5-C6-N6	12.22	133.47	123.70
22	BA	1129	A	C5-C6-N6	12.22	133.48	123.70
22	BA	1784	A	C5-C6-N6	12.21	133.47	123.70
1	AA	915	A	C5-C6-N6	12.21	133.47	123.70
22	BA	2542	A	C5-C6-N6	12.21	133.47	123.70
1	AA	572	A	C5-C6-N6	12.20	133.46	123.70
22	BA	943	A	C5-C6-N6	12.19	133.45	123.70
22	BA	1156	A	C5-C6-N6	12.19	133.46	123.70
22	BA	1515	A	C5-C6-N6	12.19	133.45	123.70
22	BA	1598	A	C5-C6-N6	12.19	133.45	123.70
22	BA	309	A	C5-C6-N6	12.18	133.45	123.70
22	BA	454	A	C5-C6-N6	12.18	133.44	123.70
1	AA	1238	A	C5-C6-N6	12.17	133.44	123.70
22	BA	905	A	C5-C6-N6	12.17	133.44	123.70
22	BA	1597	A	C5-C6-N6	12.16	133.43	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	820	A	C5-C6-N6	12.16	133.43	123.70
22	BA	497	A	C5-C6-N6	12.15	133.42	123.70
1	AA	253	A	N7-C8-N9	-12.15	107.73	113.80
1	AA	412	A	C5-C6-N6	12.15	133.42	123.70
22	BA	1127	A	C5-C6-N6	12.15	133.42	123.70
1	AA	1447	A	C5-C6-N6	12.14	133.41	123.70
22	BA	1616	A	C5-C6-N6	12.13	133.40	123.70
22	BA	2054	A	N7-C8-N9	-12.12	107.74	113.80
1	AA	1299	A	N7-C8-N9	-12.12	107.74	113.80
22	BA	1632	A	C5-C6-N6	12.12	133.40	123.70
22	BA	1655	A	C5-C6-N6	12.12	133.40	123.70
22	BA	1570	A	C5-C6-N6	12.11	133.39	123.70
22	BA	1353	A	C5-C6-N6	12.11	133.39	123.70
1	AA	1500	A	C5-C6-N6	12.11	133.39	123.70
22	BA	1899	A	C5-C6-N6	12.10	133.38	123.70
1	AA	152	A	C5-C6-N6	12.10	133.38	123.70
22	BA	111	A	C5-C6-N6	12.10	133.38	123.70
22	BA	2297	A	C5-C6-N6	12.09	133.37	123.70
1	AA	900	A	C5-C6-N6	12.08	133.36	123.70
1	AA	195	A	C5-C6-N6	12.07	133.36	123.70
22	BA	10	A	C5-C6-N6	12.07	133.35	123.70
55	B8	42	A	N7-C8-N9	-12.06	107.77	113.80
22	BA	191	A	C5-C6-N6	12.05	133.34	123.70
22	BA	2565	A	C5-C6-N6	12.05	133.34	123.70
22	BA	1427	A	C5-C6-N6	12.03	133.32	123.70
22	BA	2268	A	C5-C6-N6	12.03	133.32	123.70
22	BA	2518	A	N7-C8-N9	-12.03	107.78	113.80
22	BA	2352	A	C5-C6-N6	12.03	133.32	123.70
1	AA	196	A	C5-C6-N6	12.02	133.32	123.70
23	BB	53	A	C5-C6-N6	12.02	133.32	123.70
1	AA	1398	A	C5-C6-N6	12.02	133.31	123.70
22	BA	1001	A	C5-C6-N6	12.02	133.31	123.70
22	BA	1272	A	C5-C6-N6	12.02	133.31	123.70
22	BA	443	A	C5-C6-N6	12.01	133.31	123.70
1	AA	1004	A	C5-C6-N6	12.01	133.31	123.70
22	BA	270	A	C5-C6-N6	12.01	133.31	123.70
22	BA	1495	A	C5-C6-N6	12.00	133.30	123.70
22	BA	83	A	C5-C6-N6	12.00	133.30	123.70
1	AA	676	A	C5-C6-N6	11.99	133.30	123.70
1	AA	151	A	C5-C6-N6	11.99	133.29	123.70
22	BA	1808	A	C5-C6-N6	11.99	133.29	123.70
1	AA	673	A	N3-C4-C5	-11.99	118.41	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	753	A	C5-C6-N6	11.99	133.29	123.70
22	BA	2266	A	C5-C6-N6	11.98	133.29	123.70
55	B8	59	A	N7-C8-N9	-11.98	107.81	113.80
1	AA	129	A	C5-C6-N6	11.98	133.28	123.70
22	BA	2198	A	C5-C6-N6	11.98	133.28	123.70
1	AA	363	A	C5-C6-N6	11.98	133.28	123.70
1	AA	768	A	C5-C6-N6	11.98	133.28	123.70
22	BA	1614	A	C5-C6-N6	11.98	133.28	123.70
22	BA	2439	A	C5-C6-N6	11.97	133.28	123.70
22	BA	1327	A	C5-C6-N6	11.97	133.28	123.70
22	BA	1755	A	C5-C6-N6	11.97	133.27	123.70
1	AA	411	A	N7-C8-N9	-11.96	107.82	113.80
1	AA	1239	A	N7-C8-N9	-11.96	107.82	113.80
22	BA	2639	A	C5-C6-N6	11.96	133.27	123.70
1	AA	915	A	N7-C8-N9	-11.96	107.82	113.80
1	AA	482	A	C5-C6-N6	11.95	133.26	123.70
1	AA	149	A	C5-C6-N6	11.94	133.25	123.70
1	AA	59	A	C5-C6-N6	11.94	133.25	123.70
22	BA	1029	A	C5-C6-N6	11.94	133.25	123.70
22	BA	2682	A	C5-C6-N6	11.93	133.25	123.70
1	AA	1446	A	N3-C4-C5	-11.93	118.45	126.80
55	B8	69	A	N7-C8-N9	-11.93	107.84	113.80
22	BA	71	A	N7-C8-N9	-11.92	107.84	113.80
22	BA	2212	A	C5-C6-N6	11.92	133.24	123.70
55	B8	73	A	N7-C8-N9	-11.92	107.84	113.80
22	BA	1342	A	C5-C6-N6	11.92	133.24	123.70
22	BA	199	A	C5-C6-N6	11.92	133.24	123.70
1	AA	906	A	C5-C6-N6	11.91	133.23	123.70
1	AA	374	A	C5-C6-N6	11.91	133.23	123.70
1	AA	1092	A	C5-C6-N6	11.91	133.23	123.70
22	BA	655	A	C5-C6-N6	11.91	133.23	123.70
22	BA	1353	A	N7-C8-N9	-11.91	107.84	113.80
1	AA	1287	A	C5-C6-N6	11.90	133.22	123.70
55	B8	76	A	N7-C8-N9	-11.90	107.85	113.80
1	AA	1179	A	C5-C6-N6	11.89	133.21	123.70
22	BA	988	A	C5-C6-N6	11.89	133.21	123.70
1	AA	371	A	N7-C8-N9	-11.88	107.86	113.80
22	BA	788	A	C5-C6-N6	11.88	133.20	123.70
22	BA	91	A	C5-C6-N6	11.87	133.20	123.70
22	BA	2602	A	N7-C8-N9	-11.87	107.86	113.80
22	BA	371	A	C5-C6-N6	11.87	133.19	123.70
22	BA	340	A	C5-C6-N6	11.86	133.19	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	81	A	C5-C6-N6	11.86	133.19	123.70
1	AA	179	A	C5-C6-N6	11.86	133.19	123.70
1	AA	119	A	C5-C6-N6	11.86	133.19	123.70
22	BA	492	A	C5-C6-N6	11.86	133.19	123.70
22	BA	1439	A	C5-C6-N6	11.86	133.18	123.70
22	BA	2433	A	N7-C8-N9	-11.85	107.87	113.80
1	AA	172	A	C5-C6-N6	11.85	133.18	123.70
22	BA	279	A	C5-C6-N6	11.84	133.17	123.70
1	AA	1456	A	C5-C6-N6	11.84	133.17	123.70
22	BA	2670	A	N7-C8-N9	-11.84	107.88	113.80
23	BB	101	A	N1-C2-N3	-11.84	123.38	129.30
22	BA	727	A	C5-C6-N6	11.83	133.17	123.70
22	BA	1928	A	C5-C6-N6	11.83	133.16	123.70
22	BA	602	A	C5-C6-N6	11.83	133.16	123.70
1	AA	26	A	C5-C6-N6	11.82	133.16	123.70
1	AA	1447	A	N7-C8-N9	-11.82	107.89	113.80
23	BB	109	A	C5-C6-N6	11.82	133.16	123.70
22	BA	2199	A	C5-C6-N6	11.82	133.16	123.70
22	BA	643	A	N7-C8-N9	-11.82	107.89	113.80
22	BA	1385	A	C5-C6-N6	11.82	133.16	123.70
1	AA	975	A	C5-C6-N6	11.81	133.15	123.70
22	BA	332	A	C5-C6-N6	11.81	133.15	123.70
22	BA	1927	A	C5-C6-N6	11.81	133.15	123.70
22	BA	2541	A	C5-C6-N6	11.81	133.15	123.70
22	BA	1032	A	C5-C6-N6	11.81	133.15	123.70
22	BA	28	A	C5-C6-N6	11.81	133.15	123.70
1	AA	918	A	C5-C6-N6	11.80	133.14	123.70
1	AA	397	A	N3-C4-C5	-11.80	118.54	126.80
22	BA	1701	A	C5-C6-N6	11.80	133.14	123.70
22	BA	1392	A	C5-C6-N6	11.79	133.14	123.70
1	AA	1476	A	C5-C6-N6	11.79	133.13	123.70
22	BA	1378	A	C5-C6-N6	11.79	133.13	123.70
22	BA	1226	A	C5-C6-N6	11.79	133.13	123.70
22	BA	788	A	N7-C8-N9	-11.79	107.91	113.80
22	BA	2566	A	C5-C6-N6	11.78	133.12	123.70
22	BA	2657	A	C5-C6-N6	11.78	133.12	123.70
22	BA	1912	A	C5-C6-N6	11.78	133.12	123.70
22	BA	783	A	N3-C4-C5	-11.77	118.56	126.80
1	AA	909	A	C5-C6-N6	11.76	133.11	123.70
22	BA	1086	A	C5-C6-N6	11.76	133.11	123.70
22	BA	532	A	C5-C6-N6	11.76	133.10	123.70
22	BA	1913	A	N7-C8-N9	-11.75	107.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1566	A	N7-C8-N9	-11.75	107.93	113.80
1	AA	1269	A	C5-C6-N6	11.74	133.10	123.70
1	AA	8	A	N7-C8-N9	-11.74	107.93	113.80
1	AA	461	A	N3-C4-C5	-11.73	118.59	126.80
55	B8	38	A	N7-C8-N9	-11.73	107.93	113.80
1	AA	1248	A	C5-C6-N6	11.73	133.08	123.70
22	BA	71	A	C5-C6-N6	11.72	133.08	123.70
22	BA	2829	A	C5-C6-N6	11.72	133.08	123.70
1	AA	44	A	C5-C6-N6	11.72	133.07	123.70
22	BA	346	A	C5-C6-N6	11.72	133.07	123.70
22	BA	1165	A	C5-C6-N6	11.72	133.07	123.70
1	AA	913	A	C5-C6-N6	11.71	133.07	123.70
22	BA	1773	A	C5-C6-N6	11.71	133.07	123.70
22	BA	2062	A	C5-C6-N6	11.71	133.07	123.70
22	BA	1586	A	C5-C6-N6	11.71	133.06	123.70
22	BA	789	A	C5-C6-N6	11.70	133.06	123.70
22	BA	2335	A	C5-C6-N6	11.70	133.06	123.70
22	BA	2211	A	C5-C6-N6	11.70	133.06	123.70
1	AA	1016	A	C5-C6-N6	11.69	133.06	123.70
22	BA	819	A	C5-C6-N6	11.69	133.05	123.70
1	AA	1513	A	C5-C6-N6	11.69	133.05	123.70
22	BA	222	A	C5-C6-N6	11.69	133.05	123.70
23	BB	58	A	C5-C6-N6	11.68	133.05	123.70
1	AA	1145	A	C5-C6-N6	11.68	133.04	123.70
22	BA	1672	A	C5-C6-N6	11.68	133.04	123.70
1	AA	959	A	C5-C6-N6	11.68	133.04	123.70
22	BA	631	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	149	A	C5-C6-N6	11.68	133.04	123.70
22	BA	2497	A	C5-C6-N6	11.68	133.04	123.70
22	BA	794	A	N3-C4-C5	-11.67	118.63	126.80
22	BA	945	A	C5-C6-N6	11.67	133.04	123.70
23	BB	99	A	C5-C6-N6	11.67	133.04	123.70
22	BA	1610	A	C5-C6-N6	11.67	133.03	123.70
22	BA	127	A	C5-C6-N6	11.66	133.03	123.70
22	BA	1073	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	815	A	C5-C6-N6	11.65	133.02	123.70
22	BA	677	A	N3-C4-C5	-11.65	118.64	126.80
22	BA	1084	A	C5-C6-N6	11.65	133.02	123.70
22	BA	2411	A	C5-C6-N6	11.65	133.02	123.70
1	AA	74	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	1936	A	N3-C4-C5	-11.65	118.64	126.80
2	AB	205	ASP	CB-CG-OD2	-11.65	107.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1301	A	C5-C6-N6	11.65	133.02	123.70
1	AA	408	A	C5-C6-N6	11.64	133.01	123.70
1	AA	996	A	N7-C8-N9	-11.64	107.98	113.80
23	BB	78	A	C5-C6-N6	11.64	133.01	123.70
22	BA	449	A	N3-C4-C5	-11.63	118.66	126.80
22	BA	1780	A	C5-C6-N6	11.63	133.01	123.70
1	AA	1346	A	C5-C6-N6	11.63	133.00	123.70
22	BA	2191	A	C5-C6-N6	11.63	133.00	123.70
22	BA	423	A	C5-C6-N6	11.63	133.00	123.70
22	BA	1069	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	243	A	C5-C6-N6	11.62	133.00	123.70
1	AA	432	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	1762	A	C5-C6-N6	11.62	133.00	123.70
22	BA	1953	A	C5-C6-N6	11.62	133.00	123.70
1	AA	321	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	429	A	C5-C6-N6	11.62	132.99	123.70
1	AA	466	A	C5-C6-N6	11.61	132.99	123.70
22	BA	825	A	C5-C6-N6	11.61	132.99	123.70
1	AA	282	A	C5-C6-N6	11.61	132.99	123.70
22	BA	705	A	N3-C4-C5	-11.61	118.67	126.80
1	AA	825	A	C5-C6-N6	11.61	132.99	123.70
22	BA	2198	A	N7-C8-N9	-11.61	108.00	113.80
22	BA	2298	A	C5-C6-N6	11.60	132.98	123.70
22	BA	322	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	609	A	C5-C6-N6	11.60	132.98	123.70
22	BA	821	A	C5-C6-N6	11.60	132.98	123.70
22	BA	231	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	1810	A	N3-C4-C5	-11.60	118.68	126.80
22	BA	2434	A	C5-C6-N6	11.60	132.98	123.70
22	BA	627	A	C5-C6-N6	11.59	132.97	123.70
22	BA	1637	A	C5-C6-N6	11.59	132.97	123.70
1	AA	1022	A	C5-C6-N6	11.59	132.97	123.70
22	BA	637	A	C5-C6-N6	11.59	132.97	123.70
22	BA	1103	A	C5-C6-N6	11.58	132.97	123.70
1	AA	1434	A	C5-C6-N6	11.58	132.97	123.70
1	AA	583	A	C5-C6-N6	11.57	132.96	123.70
23	BB	29	A	C5-C6-N6	11.57	132.95	123.70
55	B8	26	A	N7-C8-N9	-11.57	108.02	113.80
1	AA	478	A	C5-C6-N6	11.56	132.95	123.70
1	AA	935	A	C5-C6-N6	11.56	132.95	123.70
22	BA	866	A	C5-C6-N6	11.56	132.95	123.70
1	AA	383	A	C4-C5-C6	11.56	122.78	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	459	A	N3-C4-C5	-11.56	118.71	126.80
22	BA	538	A	C5-C6-N6	11.56	132.94	123.70
1	AA	44	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	171	A	C5-C6-N6	11.55	132.94	123.70
1	AA	1130	A	C5-C6-N6	11.55	132.94	123.70
22	BA	104	A	C5-C6-N6	11.55	132.94	123.70
22	BA	802	A	C5-C6-N6	11.55	132.94	123.70
1	AA	766	A	C5-C6-N6	11.55	132.94	123.70
55	B8	21	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	787	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	2781	A	C5-C6-N6	11.54	132.94	123.70
1	AA	533	A	N3-C4-C5	-11.54	118.72	126.80
1	AA	1480	A	C5-C6-N6	11.54	132.93	123.70
22	BA	2748	A	C5-C6-N6	11.54	132.94	123.70
1	AA	1275	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	1322	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1441	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	1650	A	N3-C4-C5	-11.54	118.72	126.80
22	BA	2281	A	N3-C4-C5	-11.54	118.72	126.80
22	BA	1525	A	C5-C6-N6	11.54	132.93	123.70
22	BA	1525	A	N7-C8-N9	-11.53	108.03	113.80
22	BA	2270	A	C5-C6-N6	11.54	132.93	123.70
22	BA	2733	A	C5-C6-N6	11.53	132.93	123.70
22	BA	402	A	C5-C6-N6	11.53	132.93	123.70
1	AA	1180	A	C5-C6-N6	11.53	132.92	123.70
1	AA	1329	A	N7-C8-N9	-11.53	108.04	113.80
22	BA	2134	A	C5-C6-N6	11.53	132.92	123.70
22	BA	899	A	C5-C6-N6	11.53	132.92	123.70
22	BA	2227	A	N7-C8-N9	-11.53	108.04	113.80
22	BA	1522	A	C5-C6-N6	11.53	132.92	123.70
22	BA	2287	A	N7-C8-N9	-11.53	108.04	113.80
22	BA	608	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	1802	A	C5-C6-N6	11.52	132.92	123.70
22	BA	2119	A	C5-C6-N6	11.52	132.92	123.70
22	BA	1069	A	C5-C6-N6	11.52	132.92	123.70
1	AA	182	A	C5-C6-N6	11.52	132.91	123.70
22	BA	1634	A	C5-C6-N6	11.52	132.91	123.70
1	AA	7	A	C5-C6-N6	11.52	132.91	123.70
22	BA	2173	A	C5-C6-N6	11.52	132.91	123.70
22	BA	204	A	C5-C6-N6	11.51	132.91	123.70
22	BA	320	A	C5-C6-N6	11.51	132.91	123.70
1	AA	60	A	C5-C6-N6	11.51	132.91	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	465	A	C8-N9-C4	11.51	110.40	105.80
22	BA	877	A	C5-C6-N6	11.50	132.90	123.70
22	BA	1321	A	C5-C6-N6	11.50	132.90	123.70
22	BA	1070	A	C5-C6-N6	11.50	132.90	123.70
1	AA	1499	A	C5-C6-N6	11.50	132.90	123.70
22	BA	2119	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	2147	A	C5-C6-N6	11.50	132.90	123.70
22	BA	49	A	C5-C6-N6	11.49	132.90	123.70
1	AA	1067	A	C5-C6-N6	11.49	132.89	123.70
22	BA	422	A	N3-C4-C5	-11.49	118.75	126.80
22	BA	981	A	C5-C6-N6	11.49	132.89	123.70
1	AA	559	A	C5-C6-N6	11.49	132.89	123.70
1	AA	1285	A	C5-C6-N6	11.49	132.89	123.70
22	BA	2346	A	C5-C6-N6	11.49	132.89	123.70
1	AA	1428	A	C5-C6-N6	11.48	132.89	123.70
22	BA	878	A	C5-C6-N6	11.48	132.89	123.70
22	BA	1901	A	C5-C6-N6	11.48	132.88	123.70
22	BA	2388	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	1384	A	C5-C6-N6	11.48	132.88	123.70
22	BA	2101	A	C5-C6-N6	11.48	132.88	123.70
22	BA	2879	A	C5-C6-N6	11.48	132.88	123.70
1	AA	1225	A	C5-C6-N6	11.48	132.88	123.70
1	AA	1250	A	C5-C6-N6	11.48	132.88	123.70
1	AA	781	A	C5-C6-N6	11.47	132.88	123.70
22	BA	1365	A	C5-C6-N6	11.47	132.88	123.70
1	AA	938	A	N3-C4-C5	-11.47	118.77	126.80
1	AA	621	A	C5-C6-N6	11.47	132.87	123.70
22	BA	1608	A	C5-C6-N6	11.47	132.87	123.70
22	BA	2309	A	C5-C6-N6	11.47	132.87	123.70
1	AA	1019	A	C5-C6-N6	11.46	132.87	123.70
22	BA	1142	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	596	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	94	A	C5-C6-N6	11.46	132.87	123.70
22	BA	2117	A	C5-C6-N6	11.46	132.87	123.70
22	BA	1759	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	1110	A	C5-C6-N6	11.45	132.86	123.70
1	AA	901	A	N3-C4-C5	-11.45	118.78	126.80
1	AA	1046	A	N3-C4-C5	-11.45	118.78	126.80
22	BA	2288	A	C5-C6-N6	11.45	132.86	123.70
2	AB	188	ASP	CB-CG-OD2	-11.45	108.00	118.30
22	BA	1048	A	C5-C6-N6	11.45	132.86	123.70
22	BA	2736	A	C5-C6-N6	11.45	132.86	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	342	A	C5-C6-N6	11.45	132.86	123.70
22	BA	404	A	C5-C6-N6	11.45	132.86	123.70
22	BA	1453	A	C5-C6-N6	11.45	132.86	123.70
22	BA	1579	A	C5-C6-N6	11.45	132.86	123.70
22	BA	1679	A	N3-C4-C5	-11.44	118.79	126.80
22	BA	2449	U	C5-C6-N1	-11.44	116.98	122.70
1	AA	197	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	554	A	C5-C6-N6	11.44	132.85	123.70
22	BA	1088	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	1008	A	C5-C6-N6	11.43	132.85	123.70
22	BA	1490	A	C5-C6-N6	11.43	132.85	123.70
22	BA	2837	A	C5-C6-N6	11.43	132.84	123.70
22	BA	111	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	120	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	428	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	1101	A	C5-C6-N6	11.42	132.83	123.70
22	BA	161	A	C5-C6-N6	11.41	132.83	123.70
22	BA	829	A	C5-C6-N6	11.41	132.83	123.70
1	AA	1014	A	C5-C6-N6	11.41	132.83	123.70
1	AA	1004	A	N7-C8-N9	-11.40	108.10	113.80
22	BA	1535	A	C5-C6-N6	11.40	132.82	123.70
22	BA	2727	A	N3-C4-C5	-11.40	118.82	126.80
1	AA	197	A	C5-C6-N6	11.40	132.82	123.70
1	AA	1101	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	1201	A	N3-C4-C5	-11.40	118.82	126.80
1	AA	1493	A	C5-C6-N6	11.39	132.82	123.70
22	BA	1067	A	C5-C6-N6	11.39	132.82	123.70
22	BA	2476	A	C5-C6-N6	11.39	132.82	123.70
22	BA	2059	A	C5-C6-N6	11.39	132.81	123.70
22	BA	2154	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	910	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	2799	A	N3-C4-C5	-11.39	118.83	126.80
22	BA	1669	A	N3-C4-C5	-11.38	118.83	126.80
22	BA	2340	A	N7-C8-N9	-11.38	108.11	113.80
22	BA	2547	A	C5-C6-N6	11.38	132.80	123.70
1	AA	51	A	C5-C6-N6	11.38	132.80	123.70
22	BA	204	A	N7-C8-N9	-11.37	108.11	113.80
22	BA	655	A	N7-C8-N9	-11.37	108.11	113.80
22	BA	294	A	N7-C8-N9	-11.37	108.11	113.80
22	BA	2809	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	547	A	C5-C6-N6	11.36	132.79	123.70
22	BA	716	A	C5-C6-N6	11.36	132.79	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	448	A	C5-C6-N6	11.36	132.79	123.70
1	AA	499	A	N7-C8-N9	-11.36	108.12	113.80
1	AA	642	A	C5-C6-N6	11.36	132.78	123.70
22	BA	1254	A	C5-C6-N6	11.35	132.78	123.70
1	AA	414	A	C5-C6-N6	11.35	132.78	123.70
1	AA	572	A	N7-C8-N9	-11.35	108.13	113.80
22	BA	892	A	C5-C6-N6	11.35	132.78	123.70
1	AA	792	A	C5-C6-N6	11.34	132.77	123.70
22	BA	347	A	C5-C6-N6	11.34	132.77	123.70
22	BA	1268	A	C5-C6-N6	11.34	132.77	123.70
22	BA	2471	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	320	A	C5-C6-N6	11.34	132.77	123.70
1	AA	468	A	N7-C8-N9	-11.34	108.13	113.80
22	BA	279	A	N7-C8-N9	-11.34	108.13	113.80
55	B8	21	A	C5-C6-N6	11.34	132.77	123.70
22	BA	2883	A	N7-C8-N9	-11.34	108.13	113.80
22	BA	670	A	C5-C6-N6	11.34	132.77	123.70
1	AA	1311	A	C5-C6-N6	11.33	132.77	123.70
22	BA	547	A	C5-C6-N6	11.33	132.77	123.70
22	BA	74	A	C5-C6-N6	11.33	132.76	123.70
1	AA	1196	A	N7-C8-N9	-11.33	108.14	113.80
22	BA	2311	A	C5-C6-N6	11.32	132.76	123.70
1	AA	32	A	N3-C4-C5	-11.32	118.88	126.80
22	BA	689	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	1189	A	N3-C4-C5	-11.32	118.88	126.80
22	BA	1504	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	84	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	2095	A	C5-C6-N6	11.32	132.75	123.70
22	BA	401	A	C5-C6-N6	11.32	132.75	123.70
22	BA	1367	A	C5-C6-N6	11.32	132.75	123.70
22	BA	1089	A	N7-C8-N9	-11.31	108.14	113.80
22	BA	1175	A	C5-C6-N6	11.31	132.75	123.70
22	BA	2792	A	N7-C8-N9	-11.31	108.14	113.80
22	BA	1785	A	C5-C6-N6	11.31	132.75	123.70
22	BA	1916	A	C5-C6-N6	11.31	132.75	123.70
22	BA	2632	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	161	A	C5-C6-N6	11.31	132.75	123.70
1	AA	1333	A	C5-C6-N6	11.31	132.75	123.70
1	AA	1188	A	C5-C6-N6	11.30	132.74	123.70
1	AA	782	A	C5-C6-N6	11.30	132.74	123.70
22	BA	2766	A	N3-C4-C5	-11.30	118.89	126.80
22	BA	2117	A	N7-C8-N9	-11.30	108.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1272	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	1603	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	2453	A	C5-C6-N6	11.30	132.74	123.70
22	BA	2887	A	C5-C6-N6	11.30	132.74	123.70
1	AA	205	A	C5-C6-N6	11.30	132.74	123.70
22	BA	2564	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	144	A	N7-C8-N9	-11.29	108.15	113.80
22	BA	925	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	1307	A	C5-C6-N6	11.30	132.74	123.70
22	BA	2430	A	C2-N3-C4	11.29	116.25	110.60
1	AA	26	A	N7-C8-N9	-11.29	108.15	113.80
1	AA	1204	A	N7-C8-N9	-11.29	108.16	113.80
22	BA	910	A	C5-C6-N6	11.29	132.73	123.70
22	BA	1111	A	N7-C8-N9	-11.29	108.16	113.80
1	AA	309	A	N7-C8-N9	-11.29	108.16	113.80
22	BA	706	A	C5-C6-N6	11.28	132.73	123.70
22	BA	1912	A	N7-C8-N9	-11.29	108.16	113.80
1	AA	55	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	590	A	C5-C6-N6	11.28	132.72	123.70
22	BA	2412	A	C5-C6-N6	11.28	132.72	123.70
1	AA	1377	A	C5-C6-N6	11.28	132.72	123.70
22	BA	603	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	1987	A	N7-C8-N9	-11.28	108.16	113.80
1	AA	595	A	C5-C6-N6	11.28	132.72	123.70
22	BA	1504	A	C5-C6-N6	11.28	132.72	123.70
22	BA	2482	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	802	A	N3-C4-C5	-11.27	118.91	126.80
22	BA	1819	A	N3-C4-C5	-11.27	118.91	126.80
22	BA	2632	A	C5-C6-N6	11.27	132.72	123.70
1	AA	263	A	C5-C6-N6	11.27	132.71	123.70
1	AA	364	A	C5-C6-N6	11.26	132.71	123.70
1	AA	969	A	C5-C6-N6	11.26	132.71	123.70
22	BA	368	A	C5-C6-N6	11.26	132.71	123.70
1	AA	1167	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	1046	A	C5-C6-N6	11.26	132.71	123.70
22	BA	1287	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	2418	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	2589	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	1847	A	C5-C6-N6	11.26	132.70	123.70
22	BA	131	A	N3-C4-C5	-11.25	118.92	126.80
1	AA	1256	A	N7-C8-N9	-11.25	108.17	113.80
22	BA	572	A	N3-C4-C5	-11.25	118.92	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2080	A	N3-C4-C5	-11.25	118.92	126.80
1	AA	246	A	N7-C8-N9	-11.25	108.18	113.80
22	BA	2101	A	N7-C8-N9	-11.25	108.18	113.80
22	BA	2459	A	N7-C8-N9	-11.24	108.18	113.80
1	AA	878	A	C5-C6-N6	11.24	132.69	123.70
22	BA	1213	A	N3-C4-C5	-11.24	118.93	126.80
22	BA	1246	A	C5-C6-N6	11.24	132.69	123.70
22	BA	2328	A	C5-C6-N6	11.24	132.69	123.70
22	BA	2541	A	N7-C8-N9	-11.24	108.18	113.80
22	BA	1260	A	C5-C6-N6	11.24	132.69	123.70
22	BA	101	A	N3-C4-C5	-11.23	118.94	126.80
22	BA	633	A	C5-C6-N6	11.23	132.69	123.70
22	BA	1583	A	C5-C6-N6	11.23	132.69	123.70
22	BA	1858	A	C5-C6-N6	11.23	132.68	123.70
22	BA	482	A	N3-C4-C5	-11.23	118.94	126.80
22	BA	820	A	N3-C4-C5	-11.23	118.94	126.80
22	BA	1304	A	N7-C8-N9	-11.23	108.19	113.80
1	AA	1340	A	C5-C6-N6	11.22	132.68	123.70
22	BA	195	A	C5-C6-N6	11.22	132.68	123.70
22	BA	1194	A	C5-C6-N6	11.22	132.68	123.70
1	AA	1377	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	2814	A	C5-C6-N6	11.22	132.68	123.70
22	BA	1744	A	C5-C6-N6	11.22	132.67	123.70
1	AA	349	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	1652	A	C5-C6-N6	11.21	132.67	123.70
22	BA	1626	A	N7-C8-N9	-11.21	108.19	113.80
22	BA	282	A	N7-C8-N9	-11.21	108.19	113.80
22	BA	1453	A	N7-C8-N9	-11.21	108.19	113.80
1	AA	1151	A	N7-C8-N9	-11.21	108.19	113.80
1	AA	190	A	N3-C4-C5	-11.21	118.95	126.80
22	BA	689	A	N3-C4-C5	-11.21	118.95	126.80
1	AA	1213	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	1678	A	C5-C6-N6	11.21	132.66	123.70
1	AA	1035	A	C5-C6-N6	11.20	132.66	123.70
1	AA	74	A	C5-C6-N6	11.20	132.66	123.70
22	BA	447	A	C5-C6-N6	11.20	132.66	123.70
1	AA	1349	A	C5-C6-N6	11.20	132.66	123.70
1	AA	143	A	C5-C6-N6	11.20	132.66	123.70
1	AA	414	A	N7-C8-N9	-11.19	108.20	113.80
1	AA	908	A	C5-C6-N6	11.19	132.66	123.70
22	BA	2530	A	C5-C6-N6	11.19	132.66	123.70
22	BA	2850	A	C5-C6-N6	11.19	132.65	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	160	A	N7-C8-N9	-11.19	108.20	113.80
22	BA	528	A	C5-C6-N6	11.19	132.65	123.70
22	BA	1077	A	C5-C6-N6	11.19	132.65	123.70
22	BA	2281	A	C5-C6-N6	11.19	132.65	123.70
22	BA	2392	A	C5-C6-N6	11.19	132.65	123.70
1	AA	814	A	C5-C6-N6	11.19	132.65	123.70
23	BB	119	A	N7-C8-N9	-11.19	108.21	113.80
1	AA	383	A	N3-C4-C5	-11.18	118.97	126.80
1	AA	1080	A	C5-C6-N6	11.18	132.65	123.70
22	BA	1385	A	N7-C8-N9	-11.18	108.21	113.80
22	BA	1609	A	N7-C8-N9	-11.18	108.21	113.80
1	AA	7	A	N7-C8-N9	-11.18	108.21	113.80
22	BA	676	A	C5-C6-N6	11.18	132.64	123.70
22	BA	1772	A	C5-C6-N6	11.18	132.64	123.70
22	BA	1583	A	N7-C8-N9	-11.18	108.21	113.80
22	BA	1169	A	N7-C8-N9	-11.17	108.21	113.80
1	AA	1081	A	N7-C8-N9	-11.17	108.21	113.80
22	BA	1698	A	C5-C6-N6	11.17	132.64	123.70
22	BA	547	A	N7-C8-N9	-11.17	108.22	113.80
1	AA	675	A	C5-C6-N6	11.17	132.63	123.70
22	BA	2126	A	C5-C6-N6	11.17	132.63	123.70
22	BA	1978	A	N7-C8-N9	-11.17	108.22	113.80
1	AA	8	A	C5-C6-N6	11.16	132.63	123.70
1	AA	1246	A	C5-C6-N6	11.16	132.63	123.70
22	BA	959	A	C5-C6-N6	11.16	132.63	123.70
22	BA	2009	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	2821	A	N7-C8-N9	-11.16	108.22	113.80
1	AA	366	A	C5-C6-N6	11.16	132.63	123.70
1	AA	787	A	C5-C6-N6	11.16	132.63	123.70
1	AA	1150	A	C5-C6-N6	11.16	132.63	123.70
22	BA	391	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	1086	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	1717	A	C5-C6-N6	11.16	132.63	123.70
22	BA	1757	A	C5-C6-N6	11.16	132.63	123.70
23	BB	45	A	C5-C6-N6	11.15	132.62	123.70
22	BA	191	A	N3-C4-C5	-11.15	118.99	126.80
22	BA	1998	A	N3-C4-C5	-11.15	118.99	126.80
1	AA	320	A	N7-C8-N9	-11.15	108.23	113.80
1	AA	353	A	N7-C8-N9	-11.15	108.23	113.80
1	AA	695	A	C5-C6-N6	11.15	132.62	123.70
22	BA	2071	A	C5-C6-N6	11.15	132.62	123.70
22	BA	226	A	C5-C6-N6	11.14	132.62	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2051	A	C5-C6-N6	11.14	132.62	123.70
22	BA	2516	A	C5-C6-N6	11.14	132.62	123.70
22	BA	1262	A	C5-C6-N6	11.14	132.61	123.70
1	AA	777	A	N7-C8-N9	-11.14	108.23	113.80
1	AA	502	A	N3-C4-C5	-11.14	119.00	126.80
1	AA	1280	A	C5-C6-N6	11.14	132.61	123.70
22	BA	1090	A	N7-C8-N9	-11.14	108.23	113.80
22	BA	1147	A	N7-C8-N9	-11.14	108.23	113.80
22	BA	1046	A	N7-C8-N9	-11.13	108.23	113.80
22	BA	2851	A	N7-C8-N9	-11.13	108.23	113.80
1	AA	306	A	C5-C6-N6	11.13	132.60	123.70
1	AA	949	A	C5-C6-N6	11.13	132.60	123.70
1	AA	1433	A	C5-C6-N6	11.13	132.60	123.70
22	BA	1952	A	N7-C8-N9	-11.13	108.23	113.80
1	AA	1204	A	C5-C6-N6	11.13	132.60	123.70
1	AA	1019	A	N7-C8-N9	-11.13	108.24	113.80
22	BA	1505	A	N7-C8-N9	-11.13	108.24	113.80
22	BA	374	A	C5-C6-N6	11.12	132.60	123.70
54	B7	9	A	C5-C6-N6	11.12	132.60	123.70
1	AA	1299	A	N3-C4-C5	-11.12	119.01	126.80
22	BA	1269	A	C5-C6-N6	11.12	132.60	123.70
1	AA	958	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	479	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	1039	A	C5-C6-N6	11.12	132.60	123.70
22	BA	2406	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	501	A	C5-C6-N6	11.12	132.59	123.70
22	BA	167	A	C5-C6-N6	11.12	132.59	123.70
22	BA	2665	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	1503	A	N7-C8-N9	-11.12	108.24	113.80
1	AA	344	A	C5-C6-N6	11.11	132.59	123.70
22	BA	2135	A	C5-C6-N6	11.11	132.59	123.70
22	BA	2738	A	C5-C6-N6	11.11	132.59	123.70
1	AA	1319	A	C5-C6-N6	11.11	132.59	123.70
22	BA	715	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	2169	A	C5-C6-N6	11.11	132.59	123.70
1	AA	495	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	1070	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	2682	A	N7-C8-N9	-11.11	108.25	113.80
1	AA	493	A	C5-C6-N6	11.10	132.58	123.70
1	AA	499	A	C5-C6-N6	11.10	132.58	123.70
22	BA	1095	A	C5-C6-N6	11.10	132.58	123.70
22	BA	1580	A	C5-C6-N6	11.10	132.58	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	265	A	C5-C6-N6	11.10	132.58	123.70
22	BA	1470	A	N3-C4-C5	-11.10	119.03	126.80
22	BA	2163	A	C5-C6-N6	11.10	132.58	123.70
22	BA	262	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	504	A	C5-C6-N6	11.10	132.58	123.70
1	AA	1360	A	C5-C6-N6	11.09	132.57	123.70
1	AA	1430	A	C5-C6-N6	11.09	132.57	123.70
22	BA	503	A	C5-C6-N6	11.09	132.57	123.70
22	BA	2531	A	N7-C8-N9	-11.09	108.25	113.80
22	BA	928	A	C5-C6-N6	11.09	132.57	123.70
22	BA	2388	A	C5-C6-N6	11.09	132.57	123.70
1	AA	535	A	C5-C6-N6	11.09	132.57	123.70
22	BA	2336	A	C5-C6-N6	11.09	132.57	123.70
22	BA	1876	A	N7-C8-N9	-11.09	108.26	113.80
22	BA	2052	A	C5-C6-N6	11.09	132.57	123.70
22	BA	2602	A	C5-C6-N6	11.09	132.57	123.70
22	BA	716	A	N7-C8-N9	-11.08	108.26	113.80
22	BA	1490	A	N7-C8-N9	-11.08	108.26	113.80
1	AA	702	A	C5-C6-N6	11.08	132.56	123.70
1	AA	1169	A	C5-C6-N6	11.08	132.56	123.70
1	AA	1246	A	N7-C8-N9	-11.08	108.26	113.80
22	BA	1427	A	N7-C8-N9	-11.08	108.26	113.80
22	BA	1548	A	N7-C8-N9	-11.08	108.26	113.80
22	BA	2725	A	N7-C8-N9	-11.08	108.26	113.80
22	BA	792	A	N7-C8-N9	-11.07	108.26	113.80
1	AA	1227	A	C5-C6-N6	11.07	132.56	123.70
22	BA	1630	A	N7-C8-N9	-11.07	108.27	113.80
22	BA	223	A	N7-C8-N9	-11.07	108.27	113.80
22	BA	262	A	C5-C6-N6	11.07	132.56	123.70
22	BA	637	A	N7-C8-N9	-11.07	108.27	113.80
22	BA	1090	A	C5-C6-N6	11.07	132.56	123.70
1	AA	1413	A	C5-C6-N6	11.07	132.55	123.70
22	BA	103	A	C5-C6-N6	11.06	132.55	123.70
22	BA	1126	A	C5-C6-N6	11.06	132.55	123.70
22	BA	1532	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	2835	A	N7-C8-N9	-11.06	108.27	113.80
1	AA	845	A	C5-C6-N6	11.06	132.55	123.70
1	AA	1394	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	526	A	C5-C6-N6	11.06	132.55	123.70
22	BA	1021	A	N3-C4-C5	-11.06	119.06	126.80
1	AA	189	A	C5-C6-N6	11.06	132.55	123.70
22	BA	2284	A	N3-C4-C5	-11.06	119.06	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	72	A	C5-C6-N6	11.06	132.55	123.70
1	AA	238	A	C5-C6-N6	11.06	132.54	123.70
1	AA	432	A	C5-C6-N6	11.06	132.55	123.70
22	BA	1608	A	N3-C4-C5	-11.06	119.06	126.80
22	BA	1809	A	C5-C6-N6	11.06	132.55	123.70
22	BA	1494	A	C5-C6-N6	11.05	132.54	123.70
1	AA	1437	A	N7-C8-N9	-11.05	108.28	113.80
22	BA	478	A	N3-C4-C5	-11.05	119.06	126.80
22	BA	513	A	N3-C4-C5	-11.05	119.06	126.80
22	BA	1144	A	C5-C6-N6	11.05	132.54	123.70
22	BA	2051	A	N3-C4-C5	-11.05	119.06	126.80
1	AA	1117	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	1419	A	C5-C6-N6	11.04	132.54	123.70
1	AA	415	A	C5-C6-N6	11.04	132.53	123.70
1	AA	574	A	C5-C6-N6	11.04	132.53	123.70
1	AA	780	A	C5-C6-N6	11.04	132.53	123.70
22	BA	666	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	1885	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	1700	A	C5-C6-N6	11.04	132.53	123.70
1	AA	1042	A	C5-C6-N6	11.04	132.53	123.70
22	BA	432	A	C5-C6-N6	11.04	132.53	123.70
1	AA	1493	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	222	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	1054	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	1383	A	C5-C6-N6	11.03	132.53	123.70
1	AA	50	A	C5-C6-N6	11.03	132.52	123.70
1	AA	315	A	N7-C8-N9	-11.03	108.29	113.80
1	AA	1229	A	N7-C8-N9	-11.03	108.29	113.80
22	BA	352	A	N7-C8-N9	-11.03	108.29	113.80
22	BA	522	A	N3-C4-C5	-11.03	119.08	126.80
22	BA	1749	A	C5-C6-N6	11.03	132.52	123.70
1	AA	1000	A	N7-C8-N9	-11.03	108.29	113.80
22	BA	1321	A	N7-C8-N9	-11.03	108.29	113.80
23	BB	104	A	C5-C6-N6	11.03	132.52	123.70
1	AA	174	A	C5-C6-N6	11.02	132.52	123.70
22	BA	344	A	C5-C6-N6	11.02	132.52	123.70
22	BA	1322	A	C5-C6-N6	11.02	132.52	123.70
22	BA	614	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	384	A	C5-C6-N6	11.02	132.51	123.70
22	BA	1010	A	C5-C6-N6	11.02	132.51	123.70
22	BA	2314	A	C5-C6-N6	11.02	132.51	123.70
22	BA	2366	A	C5-C6-N6	11.02	132.51	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	640	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	819	A	N3-C4-C5	-11.01	119.09	126.80
22	BA	1918	A	C5-C6-N6	11.01	132.51	123.70
22	BA	1919	A	C5-C6-N6	11.01	132.51	123.70
1	AA	162	A	N3-C4-C5	-11.01	119.10	126.80
22	BA	1000	A	N3-C4-C5	-11.01	119.10	126.80
23	BB	108	A	C5-C6-N6	11.01	132.50	123.70
22	BA	213	A	N7-C8-N9	-11.00	108.30	113.80
1	AA	325	A	C5-C6-N6	11.00	132.50	123.70
22	BA	146	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	909	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	2278	A	C5-C6-N6	11.00	132.50	123.70
22	BA	574	A	C5-C6-N6	11.00	132.50	123.70
22	BA	896	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	905	A	N7-C8-N9	-11.00	108.30	113.80
1	AA	1329	A	C5-C6-N6	10.99	132.50	123.70
1	AA	596	A	C5-C6-N6	10.99	132.49	123.70
1	AA	978	A	N7-C8-N9	-10.99	108.30	113.80
22	BA	73	A	C5-C6-N6	10.99	132.49	123.70
22	BA	1284	A	C5-C6-N6	10.99	132.49	123.70
22	BA	2060	A	N7-C8-N9	-10.99	108.31	113.80
22	BA	1085	A	C5-C6-N6	10.99	132.49	123.70
22	BA	1858	A	N7-C8-N9	-10.99	108.31	113.80
22	BA	2062	A	N7-C8-N9	-10.99	108.31	113.80
22	BA	2176	A	C5-C6-N6	10.99	132.49	123.70
22	BA	2513	A	N3-C4-C5	-10.98	119.11	126.80
1	AA	451	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	1596	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	900	A	C5-C6-N6	10.98	132.48	123.70
22	BA	1508	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	1286	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	1877	A	C5-C6-N6	10.98	132.48	123.70
22	BA	2800	A	C5-C6-N6	10.98	132.48	123.70
1	AA	1155	A	N7-C8-N9	-10.97	108.31	113.80
22	BA	685	A	C5-C6-N6	10.97	132.48	123.70
22	BA	2227	A	C5-C6-N6	10.97	132.48	123.70
1	AA	306	A	N7-C8-N9	-10.97	108.31	113.80
22	BA	1420	A	N7-C8-N9	-10.97	108.31	113.80
1	AA	181	A	N7-C8-N9	-10.97	108.32	113.80
22	BA	1029	A	N3-C4-C5	-10.97	119.12	126.80
22	BA	1050	A	C5-C6-N6	10.97	132.47	123.70
22	BA	2376	A	C5-C6-N6	10.97	132.47	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2700	A	N3-C4-C5	-10.97	119.12	126.80
1	AA	1374	A	N7-C8-N9	-10.97	108.32	113.80
22	BA	1014	A	N7-C8-N9	-10.97	108.32	113.80
1	AA	131	A	C5-C6-N6	10.96	132.47	123.70
22	BA	2700	A	C5-C6-N6	10.96	132.47	123.70
22	BA	2778	A	C5-C6-N6	10.96	132.47	123.70
1	AA	1196	A	C5-C6-N6	10.96	132.47	123.70
1	AA	1534	A	C5-C6-N6	10.96	132.47	123.70
22	BA	1596	A	C5-C6-N6	10.96	132.47	123.70
22	BA	2381	A	N7-C8-N9	-10.96	108.32	113.80
1	AA	1289	A	C5-C6-N6	10.96	132.47	123.70
23	BB	73	A	N7-C8-N9	-10.96	108.32	113.80
1	AA	1251	A	C5-C6-N6	10.95	132.46	123.70
22	BA	1470	A	C5-C6-N6	10.96	132.46	123.70
22	BA	1783	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1	A	C5-C6-N6	10.95	132.46	123.70
1	AA	583	A	N7-C8-N9	-10.95	108.33	113.80
1	AA	968	A	C5-C6-N6	10.95	132.46	123.70
22	BA	1264	A	C5-C6-N6	10.95	132.46	123.70
22	BA	1419	A	N7-C8-N9	-10.95	108.33	113.80
1	AA	130	A	C5-C6-N6	10.95	132.46	123.70
22	BA	1503	A	C5-C6-N6	10.95	132.46	123.70
1	AA	300	A	N3-C4-C5	-10.94	119.14	126.80
1	AA	1163	A	N3-C4-C5	-10.94	119.14	126.80
22	BA	19	A	N7-C8-N9	-10.94	108.33	113.80
22	BA	2882	A	N7-C8-N9	-10.94	108.33	113.80
55	B8	14	A	C5-C6-N6	10.94	132.45	123.70
1	AA	1408	A	C5-C6-N6	10.94	132.45	123.70
22	BA	1969	A	C5-C6-N6	10.94	132.45	123.70
22	BA	2171	A	N7-C8-N9	-10.94	108.33	113.80
1	AA	563	A	N3-C4-C5	-10.94	119.15	126.80
22	BA	2377	A	N7-C8-N9	-10.94	108.33	113.80
22	BA	2654	A	C5-C6-N6	10.93	132.45	123.70
22	BA	1020	A	C5-C6-N6	10.93	132.44	123.70
22	BA	2471	A	C5-C6-N6	10.93	132.44	123.70
1	AA	143	A	N7-C8-N9	-10.93	108.34	113.80
1	AA	1531	A	C5-C6-N6	10.93	132.44	123.70
22	BA	793	A	N7-C8-N9	-10.93	108.34	113.80
22	BA	2706	A	C5-C6-N6	10.93	132.44	123.70
1	AA	1257	A	C5-C6-N6	10.92	132.44	123.70
22	BA	251	A	N3-C4-C5	-10.92	119.15	126.80
22	BA	2247	A	N3-C4-C5	-10.92	119.15	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1171	A	N3-C4-C5	-10.92	119.16	126.80
1	AA	1502	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	181	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	2163	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	2468	A	N7-C8-N9	-10.92	108.34	113.80
1	AA	1067	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	141	G	N7-C8-N9	10.92	118.56	113.10
22	BA	1347	A	C5-C6-N6	10.92	132.43	123.70
23	BB	57	A	C5-C6-N6	10.92	132.43	123.70
55	B8	66	A	N7-C8-N9	-10.92	108.34	113.80
1	AA	435	A	C5-C6-N6	10.91	132.43	123.70
1	AA	1163	A	N7-C8-N9	-10.91	108.34	113.80
22	BA	1057	A	C5-C6-N6	10.91	132.43	123.70
1	AA	553	A	N3-C4-C5	-10.91	119.16	126.80
22	BA	1302	A	N7-C8-N9	-10.91	108.34	113.80
55	B8	73	A	C5-C6-N6	10.91	132.43	123.70
22	BA	2513	A	C5-C6-N6	10.91	132.43	123.70
1	AA	313	A	N3-C4-C5	-10.91	119.16	126.80
22	BA	1509	A	N7-C8-N9	-10.91	108.35	113.80
22	BA	2740	A	C5-C6-N6	10.91	132.43	123.70
1	AA	546	A	C5-C6-N6	10.91	132.43	123.70
22	BA	1089	A	C5-C6-N6	10.91	132.43	123.70
1	AA	914	A	N7-C8-N9	-10.90	108.35	113.80
22	BA	483	A	N7-C8-N9	-10.90	108.35	113.80
1	AA	1503	A	C5-C6-N6	10.90	132.42	123.70
22	BA	721	A	N7-C8-N9	-10.90	108.35	113.80
22	BA	1241	A	N3-C4-C5	-10.90	119.17	126.80
22	BA	1403	A	N3-C4-C5	-10.90	119.17	126.80
1	AA	983	A	C5-C6-N6	10.89	132.42	123.70
1	AA	1111	A	N7-C8-N9	-10.89	108.35	113.80
22	BA	172	A	C5-C6-N6	10.89	132.42	123.70
22	BA	1739	A	C5-C6-N6	10.89	132.42	123.70
1	AA	139	A	N7-C8-N9	-10.89	108.36	113.80
17	AQ	16	LYS	CD-CE-NZ	10.89	136.75	111.70
22	BA	1275	A	N7-C8-N9	-10.89	108.36	113.80
22	BA	2134	A	N7-C8-N9	-10.89	108.36	113.80
1	AA	182	A	N7-C8-N9	-10.89	108.36	113.80
1	AA	1111	A	C5-C6-N6	10.89	132.41	123.70
1	AA	465	A	C5-C6-N6	10.89	132.41	123.70
1	AA	1499	A	N7-C8-N9	-10.89	108.36	113.80
22	BA	299	A	N7-C8-N9	-10.89	108.36	113.80
22	BA	739	A	C5-C6-N6	10.89	132.41	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	866	A	N7-C8-N9	-10.89	108.36	113.80
22	BA	2317	A	C5-C6-N6	10.88	132.41	123.70
1	AA	1410	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	654	A	N7-C8-N9	-10.88	108.36	113.80
1	AA	59	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	1635	A	C5-C6-N6	10.88	132.41	123.70
1	AA	279	A	C5-C6-N6	10.88	132.40	123.70
1	AA	600	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	324	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	1932	A	C5-C6-N6	10.88	132.40	123.70
22	BA	1759	A	C5-C6-N6	10.88	132.40	123.70
22	BA	2660	A	C5-C6-N6	10.88	132.40	123.70
1	AA	250	A	C5-C6-N6	10.87	132.40	123.70
22	BA	1359	A	C5-C6-N6	10.87	132.40	123.70
22	BA	1431	A	C5-C6-N6	10.87	132.40	123.70
22	BA	2333	A	N7-C8-N9	-10.87	108.36	113.80
1	AA	393	A	C5-C6-N6	10.87	132.40	123.70
1	AA	794	A	N7-C8-N9	-10.87	108.36	113.80
22	BA	1610	A	N7-C8-N9	-10.87	108.36	113.80
22	BA	354	A	N7-C8-N9	-10.87	108.36	113.80
22	BA	1664	A	N3-C4-C5	-10.87	119.19	126.80
22	BA	1936	A	C5-C6-N6	10.87	132.40	123.70
1	AA	349	A	C5-C6-N6	10.87	132.39	123.70
22	BA	2377	A	C5-C6-N6	10.87	132.39	123.70
1	AA	872	A	C5-C6-N6	10.86	132.39	123.70
22	BA	196	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	1552	A	C5-C6-N6	10.87	132.39	123.70
1	AA	509	A	C5-C6-N6	10.86	132.39	123.70
1	AA	1021	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	256	A	C5-C6-N6	10.86	132.39	123.70
22	BA	782	A	N3-C4-C5	-10.86	119.20	126.80
22	BA	1960	A	C5-C6-N6	10.86	132.38	123.70
22	BA	1966	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	2142	A	N3-C4-C5	-10.86	119.20	126.80
55	B8	41	A	C5-C6-N6	10.86	132.38	123.70
1	AA	353	A	C5-C6-N6	10.85	132.38	123.70
1	AA	430	A	C5-C6-N6	10.85	132.38	123.70
22	BA	2114	A	C5-C6-N6	10.85	132.38	123.70
22	BA	1998	A	C5-C6-N6	10.85	132.38	123.70
22	BA	685	A	N7-C8-N9	-10.85	108.38	113.80
22	BA	749	A	C5-C6-N6	10.85	132.38	123.70
22	BA	900	A	N7-C8-N9	-10.85	108.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	65	A	C5-C6-N6	10.85	132.38	123.70
55	B8	59	A	C5-C6-N6	10.85	132.38	123.70
22	BA	892	A	N7-C8-N9	-10.84	108.38	113.80
1	AA	336	A	C5-C6-N6	10.84	132.37	123.70
1	AA	1036	A	C5-C6-N6	10.84	132.37	123.70
22	BA	172	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	996	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	44	A	C5-C6-N6	10.84	132.37	123.70
22	BA	508	A	C5-C6-N6	10.84	132.37	123.70
1	AA	1146	A	N7-C8-N9	-10.84	108.38	113.80
1	AA	1005	A	C5-C6-N6	10.84	132.37	123.70
22	BA	1665	A	C5-C6-N6	10.84	132.37	123.70
22	BA	2314	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	42	A	C5-C6-N6	10.83	132.37	123.70
22	BA	181	A	C5-C6-N6	10.83	132.37	123.70
22	BA	1598	A	N3-C4-C5	-10.83	119.22	126.80
1	AA	313	A	C5-C6-N6	10.83	132.37	123.70
22	BA	1189	A	C5-C6-N6	10.83	132.36	123.70
22	BA	1960	A	N7-C8-N9	-10.83	108.39	113.80
1	AA	767	A	N7-C8-N9	-10.83	108.39	113.80
22	BA	644	A	N7-C8-N9	-10.83	108.39	113.80
22	BA	1088	A	C5-C6-N6	10.83	132.36	123.70
22	BA	1433	A	C5-C6-N6	10.83	132.36	123.70
22	BA	1755	A	N7-C8-N9	-10.83	108.39	113.80
22	BA	2468	A	C5-C6-N6	10.83	132.36	123.70
22	BA	734	A	N7-C8-N9	-10.82	108.39	113.80
23	BB	39	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	1853	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	1900	A	C5-C6-N6	10.82	132.36	123.70
1	AA	873	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	896	A	C5-C6-N6	10.82	132.36	123.70
22	BA	231	A	C5-C6-N6	10.82	132.35	123.70
22	BA	749	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	1505	A	C5-C6-N6	10.82	132.35	123.70
22	BA	2679	A	N3-C4-C5	-10.82	119.23	126.80
22	BA	125	A	N7-C8-N9	-10.81	108.39	113.80
22	BA	347	A	N7-C8-N9	-10.81	108.39	113.80
22	BA	750	A	N3-C4-C5	-10.81	119.23	126.80
22	BA	2170	A	C5-C6-N6	10.81	132.35	123.70
1	AA	253	A	C5-C6-N6	10.81	132.35	123.70
1	AA	663	A	N7-C8-N9	-10.81	108.39	113.80
1	AA	1500	A	N3-C4-C5	-10.81	119.23	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	330	A	N3-C4-C5	-10.81	119.23	126.80
22	BA	294	A	C5-C6-N6	10.81	132.35	123.70
1	AA	1117	A	C5-C6-N6	10.81	132.35	123.70
1	AA	1362	A	C5-C6-N6	10.81	132.35	123.70
23	BB	52	A	N7-C8-N9	-10.81	108.39	113.80
1	AA	262	A	C5-C6-N6	10.81	132.34	123.70
22	BA	2776	A	N7-C8-N9	-10.81	108.40	113.80
1	AA	747	A	C5-C6-N6	10.80	132.34	123.70
1	AA	977	A	C5-C6-N6	10.80	132.34	123.70
22	BA	1067	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	1073	A	C5-C6-N6	10.80	132.34	123.70
22	BA	528	A	N7-C8-N9	-10.80	108.40	113.80
1	AA	243	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	689	A	C5-C6-N6	10.80	132.34	123.70
1	AA	1145	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	1151	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	2765	A	C5-C6-N6	10.79	132.34	123.70
22	BA	878	A	N7-C8-N9	-10.79	108.40	113.80
1	AA	408	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	563	A	N3-C4-C5	-10.79	119.25	126.80
1	AA	327	A	N7-C8-N9	-10.79	108.41	113.80
1	AA	749	A	C5-C6-N6	10.79	132.33	123.70
22	BA	1237	A	C5-C6-N6	10.79	132.33	123.70
1	AA	892	A	C5-C6-N6	10.79	132.33	123.70
22	BA	582	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	2750	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	217	A	N3-C4-C5	-10.79	119.25	126.80
22	BA	278	A	C5-C6-N6	10.78	132.33	123.70
22	BA	936	A	N7-C8-N9	-10.78	108.41	113.80
22	BA	1285	A	N3-C4-C5	-10.79	119.25	126.80
22	BA	2757	A	N3-C4-C5	-10.78	119.25	126.80
1	AA	949	A	N7-C8-N9	-10.78	108.41	113.80
22	BA	1593	A	N7-C8-N9	-10.78	108.41	113.80
22	BA	2899	A	C5-C6-N6	10.78	132.32	123.70
1	AA	160	A	C5-C6-N6	10.78	132.32	123.70
22	BA	52	A	C5-C6-N6	10.78	132.32	123.70
22	BA	718	A	C5-C6-N6	10.78	132.32	123.70
22	BA	1009	A	C5-C6-N6	10.78	132.32	123.70
22	BA	1050	A	N7-C8-N9	-10.78	108.41	113.80
1	AA	1346	A	N7-C8-N9	-10.77	108.41	113.80
22	BA	311	A	C5-C6-N6	10.77	132.32	123.70
22	BA	1805	A	N7-C8-N9	-10.77	108.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1261	A	C5-C6-N6	10.77	132.32	123.70
1	AA	784	A	N7-C8-N9	-10.77	108.42	113.80
1	AA	860	A	N3-C4-C5	-10.77	119.26	126.80
1	AA	873	A	C5-C6-N6	10.77	132.32	123.70
1	AA	1318	A	C5-C6-N6	10.77	132.32	123.70
22	BA	1096	A	N7-C8-N9	-10.77	108.42	113.80
22	BA	1469	A	N3-C4-C5	-10.77	119.26	126.80
1	AA	456	A	N7-C8-N9	-10.77	108.42	113.80
22	BA	1194	A	N7-C8-N9	-10.77	108.42	113.80
22	BA	1342	A	N7-C8-N9	-10.77	108.42	113.80
22	BA	2080	A	C5-C6-N6	10.77	132.31	123.70
1	AA	468	A	C5-C6-N6	10.77	132.31	123.70
22	BA	804	A	N7-C8-N9	-10.77	108.42	113.80
22	BA	863	A	N3-C4-C5	-10.77	119.26	126.80
23	BB	53	A	N7-C8-N9	-10.77	108.42	113.80
22	BA	428	A	C5-C6-N6	10.76	132.31	123.70
22	BA	1308	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	1654	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	2837	A	N3-C4-C5	-10.76	119.27	126.80
22	BA	1522	A	N7-C8-N9	-10.76	108.42	113.80
1	AA	794	A	C5-C6-N6	10.76	132.31	123.70
22	BA	2158	A	C5-C6-N6	10.76	132.31	123.70
1	AA	681	A	N7-C8-N9	-10.76	108.42	113.80
1	AA	1271	A	N7-C8-N9	-10.76	108.42	113.80
1	AA	602	A	N7-C8-N9	-10.75	108.42	113.80
1	AA	687	A	C5-C6-N6	10.75	132.30	123.70
22	BA	613	A	C5-C6-N6	10.75	132.30	123.70
22	BA	1328	A	C5-C6-N6	10.75	132.30	123.70
1	AA	98	A	C5-C6-N6	10.75	132.30	123.70
1	AA	130	A	N7-C8-N9	-10.75	108.42	113.80
1	AA	151	A	N7-C8-N9	-10.75	108.42	113.80
1	AA	190	A	C4-C5-C6	10.75	122.38	117.00
1	AA	547	A	N7-C8-N9	-10.75	108.42	113.80
22	BA	2273	A	C5-C6-N6	10.75	132.30	123.70
55	B8	42	A	C5-C6-N6	10.75	132.30	123.70
1	AA	706	A	N3-C4-C5	-10.75	119.28	126.80
22	BA	1700	A	N7-C8-N9	-10.75	108.43	113.80
1	AA	712	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	89	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	1705	A	N7-C8-N9	-10.74	108.43	113.80
1	AA	356	A	N3-C4-C5	-10.74	119.28	126.80
22	BA	125	A	C5-C6-N6	10.74	132.29	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	933	A	N7-C8-N9	-10.74	108.43	113.80
1	AA	901	A	C4-C5-C6	10.74	122.37	117.00
22	BA	21	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	2019	A	C5-C6-N6	10.74	132.29	123.70
1	AA	1285	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	927	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	2736	A	N7-C8-N9	-10.74	108.43	113.80
1	AA	189	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	5	A	N7-C8-N9	-10.74	108.43	113.80
1	AA	913	A	N7-C8-N9	-10.74	108.43	113.80
1	AA	964	A	C5-C6-N6	10.74	132.29	123.70
22	BA	718	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	1801	A	C5-C6-N6	10.73	132.29	123.70
1	AA	553	A	N7-C8-N9	-10.73	108.43	113.80
1	AA	573	A	C5-C6-N6	10.73	132.29	123.70
22	BA	38	A	C5-C6-N6	10.73	132.29	123.70
22	BA	1383	A	N7-C8-N9	-10.73	108.43	113.80
1	AA	71	A	C5-C6-N6	10.73	132.29	123.70
1	AA	1289	A	N7-C8-N9	-10.73	108.43	113.80
1	AA	1333	A	N7-C8-N9	-10.73	108.43	113.80
22	BA	126	A	N7-C8-N9	-10.73	108.43	113.80
22	BA	2893	A	N7-C8-N9	-10.73	108.44	113.80
1	AA	1022	A	N7-C8-N9	-10.73	108.44	113.80
1	AA	1044	A	C5-C6-N6	10.73	132.28	123.70
1	AA	1339	A	N7-C8-N9	-10.73	108.44	113.80
22	BA	2322	A	C5-C6-N6	10.73	132.28	123.70
22	BA	2740	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	1040	A	C5-C6-N6	10.73	132.28	123.70
22	BA	2461	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	2879	A	N7-C8-N9	-10.73	108.44	113.80
1	AA	807	A	C5-C6-N6	10.72	132.28	123.70
1	AA	655	A	N7-C8-N9	-10.72	108.44	113.80
22	BA	1808	A	N7-C8-N9	-10.72	108.44	113.80
1	AA	1311	A	N7-C8-N9	-10.72	108.44	113.80
22	BA	346	A	N7-C8-N9	-10.72	108.44	113.80
1	AA	493	A	N7-C8-N9	-10.71	108.44	113.80
22	BA	104	A	N7-C8-N9	-10.71	108.44	113.80
23	BB	104	A	N7-C8-N9	-10.71	108.44	113.80
22	BA	1679	A	C5-C6-N6	10.71	132.27	123.70
22	BA	2478	A	C5-C6-N6	10.71	132.27	123.70
55	B8	14	A	N7-C8-N9	-10.71	108.44	113.80
1	AA	914	A	C5-C6-N6	10.71	132.27	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1676	A	C5-C6-N6	10.71	132.27	123.70
1	AA	53	A	N7-C8-N9	-10.71	108.45	113.80
22	BA	345	A	C5-C6-N6	10.71	132.27	123.70
22	BA	972	A	C5-C6-N6	10.71	132.27	123.70
22	BA	2082	A	C5-C6-N6	10.71	132.27	123.70
22	BA	2750	A	C5-C6-N6	10.71	132.27	123.70
1	AA	51	A	N7-C8-N9	-10.70	108.45	113.80
1	AA	1082	A	C5-C6-N6	10.71	132.26	123.70
22	BA	2547	A	N7-C8-N9	-10.71	108.45	113.80
1	AA	2	A	C5-C6-N6	10.70	132.26	123.70
1	AA	864	A	C5-C6-N6	10.70	132.26	123.70
22	BA	753	A	N3-C4-C5	-10.70	119.31	126.80
22	BA	1080	A	C5-C6-N6	10.70	132.26	123.70
22	BA	167	A	N7-C8-N9	-10.70	108.45	113.80
22	BA	1544	A	N3-C4-C5	-10.70	119.31	126.80
22	BA	1590	A	N7-C8-N9	-10.70	108.45	113.80
23	BB	29	A	N7-C8-N9	-10.70	108.45	113.80
1	AA	1368	A	C5-C6-N6	10.70	132.26	123.70
22	BA	644	A	N3-C4-C5	-10.69	119.31	126.80
22	BA	1244	A	N7-C8-N9	-10.70	108.45	113.80
22	BA	1502	A	N7-C8-N9	-10.70	108.45	113.80
22	BA	1744	A	N7-C8-N9	-10.69	108.45	113.80
1	AA	1374	A	C5-C6-N6	10.69	132.25	123.70
1	AA	1105	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	917	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	960	A	N3-C4-C5	-10.69	119.32	126.80
22	BA	2184	A	N7-C8-N9	-10.69	108.45	113.80
1	AA	560	A	N7-C8-N9	-10.69	108.46	113.80
22	BA	21	A	N3-C4-C5	-10.69	119.32	126.80
1	AA	642	A	N7-C8-N9	-10.69	108.46	113.80
22	BA	556	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	2309	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	2478	A	N7-C8-N9	-10.69	108.46	113.80
22	BA	1147	A	C5-C6-N6	10.69	132.25	123.70
22	BA	2298	A	N7-C8-N9	-10.69	108.46	113.80
22	BA	422	A	C5-C6-N6	10.68	132.25	123.70
22	BA	1096	A	C5-C6-N6	10.68	132.25	123.70
1	AA	509	A	N3-C4-C5	-10.68	119.32	126.80
19	AS	3	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	AA	609	A	C5-C6-N6	10.68	132.24	123.70
22	BA	693	A	N3-C4-C5	-10.68	119.33	126.80
1	AA	600	A	C5-C6-N6	10.68	132.24	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	176	A	N7-C8-N9	-10.68	108.46	113.80
22	BA	668	A	N7-C8-N9	-10.68	108.46	113.80
22	BA	1393	A	N7-C8-N9	-10.68	108.46	113.80
22	BA	1077	A	N7-C8-N9	-10.67	108.46	113.80
1	AA	109	A	C5-C6-N6	10.67	132.24	123.70
1	AA	974	A	C5-C6-N6	10.67	132.24	123.70
22	BA	244	A	N3-C4-C5	-10.67	119.33	126.80
22	BA	1057	A	N7-C8-N9	-10.67	108.46	113.80
1	AA	223	A	C5-C6-N6	10.67	132.24	123.70
1	AA	759	A	C5-C6-N6	10.67	132.24	123.70
1	AA	1375	A	N7-C8-N9	-10.67	108.47	113.80
22	BA	2800	A	N7-C8-N9	-10.67	108.47	113.80
23	BB	58	A	N7-C8-N9	-10.67	108.46	113.80
1	AA	935	A	N7-C8-N9	-10.67	108.47	113.80
1	AA	430	A	N7-C8-N9	-10.67	108.47	113.80
1	AA	676	A	N7-C8-N9	-10.67	108.47	113.80
1	AA	983	A	N3-C4-C5	-10.67	119.33	126.80
1	AA	746	A	N3-C4-C5	-10.66	119.33	126.80
23	BB	66	A	C5-C6-N6	10.66	132.23	123.70
1	AA	172	A	N7-C8-N9	-10.66	108.47	113.80
1	AA	205	A	N7-C8-N9	-10.66	108.47	113.80
1	AA	539	A	C5-C6-N6	10.66	132.23	123.70
1	AA	621	A	N3-C4-C5	-10.66	119.34	126.80
1	AA	1016	A	N7-C8-N9	-10.66	108.47	113.80
1	AA	675	A	N7-C8-N9	-10.66	108.47	113.80
1	AA	845	A	N7-C8-N9	-10.66	108.47	113.80
1	AA	1146	A	C5-C6-N6	10.66	132.23	123.70
1	AA	1201	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	1977	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	1640	A	N7-C8-N9	-10.65	108.47	113.80
22	BA	1885	A	C5-C6-N6	10.65	132.22	123.70
22	BA	1603	A	N3-C4-C5	-10.65	119.34	126.80
22	BA	1784	A	N7-C8-N9	-10.65	108.47	113.80
22	BA	2241	A	N3-C4-C5	-10.65	119.34	126.80
22	BA	2560	A	C5-C6-N6	10.65	132.22	123.70
22	BA	2590	A	N7-C8-N9	-10.65	108.47	113.80
1	AA	969	A	N7-C8-N9	-10.65	108.48	113.80
1	AA	1005	A	N7-C8-N9	-10.65	108.48	113.80
22	BA	2761	A	C5-C6-N6	10.65	132.22	123.70
22	BA	1028	A	C5-C6-N6	10.65	132.22	123.70
22	BA	1048	A	N3-C4-C5	-10.65	119.35	126.80
23	BB	52	A	C5-C6-N6	10.65	132.22	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	228	A	N7-C8-N9	-10.64	108.48	113.80
22	BA	432	A	N7-C8-N9	-10.64	108.48	113.80
22	BA	2114	A	N3-C4-C5	-10.64	119.35	126.80
22	BA	1535	A	N7-C8-N9	-10.64	108.48	113.80
1	AA	655	A	N3-C4-C5	-10.64	119.35	126.80
1	AA	55	A	N3-C4-C5	-10.64	119.36	126.80
1	AA	1225	A	N7-C8-N9	-10.64	108.48	113.80
22	BA	142	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	227	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	1328	A	N7-C8-N9	-10.64	108.48	113.80
22	BA	2376	A	N7-C8-N9	-10.63	108.48	113.80
1	AA	236	A	C5-C6-N6	10.63	132.21	123.70
1	AA	452	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	251	A	C4-C5-C6	10.63	122.32	117.00
1	AA	539	A	N3-C4-C5	-10.63	119.36	126.80
22	BA	2705	A	C5-C6-N6	10.63	132.21	123.70
1	AA	1150	A	N7-C8-N9	-10.63	108.48	113.80
1	AA	1171	A	C5-C6-N6	10.63	132.20	123.70
22	BA	861	A	N3-C4-C5	-10.63	119.36	126.80
22	BA	1028	A	N7-C8-N9	-10.63	108.49	113.80
22	BA	2158	A	N7-C8-N9	-10.63	108.49	113.80
22	BA	1632	A	N7-C8-N9	-10.62	108.49	113.80
22	BA	1713	A	C5-C6-N6	10.62	132.20	123.70
22	BA	207	A	N3-C4-C5	-10.62	119.36	126.80
22	BA	2031	A	N7-C8-N9	-10.62	108.49	113.80
22	BA	2267	A	N3-C4-C5	-10.62	119.36	126.80
1	AA	994	A	C5-C6-N6	10.62	132.20	123.70
22	BA	2886	A	N7-C8-N9	-10.62	108.49	113.80
1	AA	2	A	N7-C8-N9	-10.62	108.49	113.80
1	AA	192	A	C5-C6-N6	10.62	132.19	123.70
22	BA	233	A	N7-C8-N9	-10.62	108.49	113.80
22	BA	608	A	C5-C6-N6	10.62	132.19	123.70
22	BA	1871	A	C5-C6-N6	10.62	132.20	123.70
1	AA	872	A	N3-C4-C5	-10.62	119.37	126.80
22	BA	933	A	C5-C6-N6	10.62	132.19	123.70
22	BA	1040	A	N7-C8-N9	-10.62	108.49	113.80
1	AA	129	A	N7-C8-N9	-10.62	108.49	113.80
22	BA	980	A	N7-C8-N9	-10.62	108.49	113.80
22	BA	1241	A	N7-C8-N9	-10.62	108.49	113.80
22	BA	1794	A	N7-C8-N9	-10.62	108.49	113.80
22	BA	2738	A	N7-C8-N9	-10.62	108.49	113.80
1	AA	441	A	C5-C6-N6	10.61	132.19	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1350	A	C5-C6-N6	10.61	132.19	123.70
22	BA	899	A	N7-C8-N9	-10.61	108.49	113.80
22	BA	2070	A	C5-C6-N6	10.61	132.19	123.70
1	AA	1492	A	N7-C8-N9	-10.61	108.50	113.80
22	BA	244	A	C5-C6-N6	10.61	132.19	123.70
22	BA	532	A	N3-C4-C5	-10.61	119.37	126.80
22	BA	592	A	N3-C4-C5	-10.61	119.37	126.80
22	BA	2170	A	N7-C8-N9	-10.61	108.50	113.80
22	BA	2173	A	N3-C4-C5	-10.61	119.37	126.80
22	BA	614	A	C5-C6-N6	10.61	132.19	123.70
1	AA	923	A	N3-C4-C5	-10.61	119.38	126.80
1	AA	116	A	C5-C6-N6	10.61	132.18	123.70
22	BA	483	A	C5-C6-N6	10.61	132.18	123.70
22	BA	1359	A	N7-C8-N9	-10.61	108.50	113.80
22	BA	2273	A	N3-C4-C5	-10.61	119.38	126.80
23	BB	115	A	C5-C6-N6	10.61	132.18	123.70
1	AA	1254	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1509	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1598	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	1672	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	1133	A	C5-C6-N6	10.60	132.18	123.70
1	AA	451	A	C5-C6-N6	10.60	132.18	123.70
1	AA	629	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1336	A	N3-C4-C5	-10.60	119.38	126.80
1	AA	523	A	C5-C6-N6	10.60	132.18	123.70
1	AA	718	A	N3-C4-C5	-10.60	119.38	126.80
1	AA	1257	A	N7-C8-N9	-10.60	108.50	113.80
1	AA	1269	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	173	A	C5-C6-N6	10.60	132.18	123.70
1	AA	65	A	N7-C8-N9	-10.59	108.50	113.80
22	BA	789	A	N7-C8-N9	-10.59	108.50	113.80
1	AA	1169	A	N7-C8-N9	-10.59	108.50	113.80
1	AA	1288	A	C5-C6-N6	10.59	132.17	123.70
22	BA	1854	A	N3-C4-C5	-10.59	119.39	126.80
1	AA	33	A	N7-C8-N9	-10.59	108.51	113.80
1	AA	1492	A	C5-C6-N6	10.59	132.17	123.70
22	BA	89	A	C5-C6-N6	10.59	132.17	123.70
22	BA	1247	A	N7-C8-N9	-10.59	108.51	113.80
22	BA	2734	A	C5-C6-N6	10.59	132.17	123.70
22	BA	1572	A	C5-C6-N6	10.59	132.17	123.70
1	AA	80	A	C5-C6-N6	10.58	132.17	123.70
22	BA	643	A	C5-C6-N6	10.58	132.17	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	712	A	N3-C4-C5	-10.58	119.39	126.80
22	BA	13	A	N3-C4-C5	-10.58	119.39	126.80
22	BA	975	A	N3-C4-C5	-10.58	119.39	126.80
22	BA	2225	A	C5-C6-N6	10.58	132.16	123.70
1	AA	1410	A	C5-C6-N6	10.58	132.16	123.70
1	AA	1503	A	N7-C8-N9	-10.58	108.51	113.80
22	BA	5	A	N3-C4-C5	-10.58	119.39	126.80
22	BA	1287	A	C5-C6-N6	10.58	132.16	123.70
1	AA	374	A	N7-C8-N9	-10.57	108.51	113.80
22	BA	423	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	917	A	C5-C6-N6	10.57	132.16	123.70
22	BA	1260	A	N3-C4-C5	-10.57	119.40	126.80
1	AA	131	A	N7-C8-N9	-10.57	108.51	113.80
1	AA	496	A	C5-C6-N6	10.57	132.16	123.70
1	AA	553	A	C5-C6-N6	10.57	132.16	123.70
1	AA	1271	A	C5-C6-N6	10.57	132.16	123.70
22	BA	218	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	278	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	661	A	N7-C8-N9	-10.57	108.52	113.80
22	BA	845	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	1847	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	1566	A	C5-C6-N6	10.57	132.16	123.70
1	AA	1394	A	C5-C6-N6	10.57	132.15	123.70
22	BA	1244	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	2003	A	C5-C6-N6	10.57	132.15	123.70
1	AA	298	A	N7-C8-N9	-10.56	108.52	113.80
1	AA	487	A	C5-C6-N6	10.56	132.15	123.70
22	BA	1805	A	C5-C6-N6	10.56	132.15	123.70
22	BA	2432	A	C5-C6-N6	10.56	132.15	123.70
22	BA	2534	A	C5-C6-N6	10.56	132.15	123.70
1	AA	1093	A	C5-C6-N6	10.56	132.15	123.70
22	BA	64	A	C5-C6-N6	10.56	132.15	123.70
22	BA	1735	A	N7-C8-N9	-10.56	108.52	113.80
1	AA	694	A	C5-C6-N6	10.56	132.15	123.70
1	AA	728	A	C5-C6-N6	10.56	132.15	123.70
22	BA	2142	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	2662	A	C5-C6-N6	10.56	132.15	123.70
1	AA	167	A	N7-C8-N9	-10.56	108.52	113.80
1	AA	523	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	1000	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	1393	A	C5-C6-N6	10.56	132.15	123.70
22	BA	2781	A	N7-C8-N9	-10.56	108.52	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	510	A	C5-C6-N6	10.55	132.14	123.70
22	BA	362	A	N7-C8-N9	-10.55	108.52	113.80
22	BA	1144	A	N3-C4-C5	-10.56	119.41	126.80
22	BA	941	A	N7-C8-N9	-10.55	108.52	113.80
22	BA	1347	A	N7-C8-N9	-10.55	108.52	113.80
22	BA	2679	A	N7-C8-N9	-10.55	108.52	113.80
1	AA	78	A	N7-C8-N9	-10.55	108.53	113.80
1	AA	1036	A	N7-C8-N9	-10.55	108.53	113.80
22	BA	2856	A	N7-C8-N9	-10.55	108.53	113.80
1	AA	3	A	C5-C6-N6	10.54	132.13	123.70
22	BA	821	A	N7-C8-N9	-10.54	108.53	113.80
22	BA	980	A	N3-C4-C5	-10.55	119.42	126.80
1	AA	101	A	N3-C4-C5	-10.54	119.42	126.80
1	AA	825	A	N7-C8-N9	-10.54	108.53	113.80
1	AA	937	A	C5-C6-N6	10.54	132.13	123.70
1	AA	1250	A	N7-C8-N9	-10.54	108.53	113.80
1	AA	1513	A	N3-C4-C5	-10.54	119.42	126.80
22	BA	2183	A	N7-C8-N9	-10.54	108.53	113.80
22	BA	1276	A	N3-C4-C5	-10.54	119.42	126.80
1	AA	238	A	N7-C8-N9	-10.54	108.53	113.80
1	AA	495	A	C5-C6-N6	10.54	132.13	123.70
22	BA	1572	A	N3-C4-C5	-10.54	119.42	126.80
1	AA	329	A	C5-C6-N6	10.54	132.13	123.70
1	AA	974	A	N7-C8-N9	-10.54	108.53	113.80
22	BA	142	A	C5-C6-N6	10.54	132.13	123.70
22	BA	1690	A	C5-C6-N6	10.54	132.13	123.70
1	AA	975	A	N7-C8-N9	-10.53	108.53	113.80
22	BA	1890	A	N7-C8-N9	-10.54	108.53	113.80
22	BA	2761	A	N3-C4-C5	-10.54	119.42	126.80
22	BA	2706	A	N3-C4-C5	-10.53	119.43	126.80
1	AA	498	A	N7-C8-N9	-10.53	108.53	113.80
22	BA	742	A	N7-C8-N9	-10.53	108.53	113.80
22	BA	1821	A	N7-C8-N9	-10.53	108.53	113.80
22	BA	1829	A	N7-C8-N9	-10.53	108.53	113.80
22	BA	2335	A	N3-C4-C5	-10.53	119.43	126.80
1	AA	496	A	N7-C8-N9	-10.53	108.53	113.80
1	AA	1375	A	C5-C6-N6	10.53	132.12	123.70
22	BA	91	A	N7-C8-N9	-10.53	108.54	113.80
22	BA	1586	A	N7-C8-N9	-10.53	108.53	113.80
22	BA	2820	A	C5-C6-N6	10.53	132.12	123.70
1	AA	1191	A	N3-C4-C5	-10.53	119.43	126.80
22	BA	196	A	C5-C6-N6	10.53	132.12	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	920	A	C5-C6-N6	10.53	132.12	123.70
22	BA	2820	A	N7-C8-N9	-10.53	108.54	113.80
1	AA	344	A	N7-C8-N9	-10.52	108.54	113.80
1	AA	1021	A	C5-C6-N6	10.52	132.12	123.70
1	AA	1428	A	N7-C8-N9	-10.52	108.54	113.80
22	BA	352	A	C5-C6-N6	10.52	132.12	123.70
22	BA	644	A	C5-C6-N6	10.52	132.12	123.70
22	BA	2531	A	C5-C6-N6	10.52	132.12	123.70
1	AA	609	A	N7-C8-N9	-10.52	108.54	113.80
1	AA	968	A	N7-C8-N9	-10.52	108.54	113.80
22	BA	2042	A	N7-C8-N9	-10.52	108.54	113.80
22	BA	83	A	N7-C8-N9	-10.52	108.54	113.80
22	BA	221	A	C5-C6-N6	10.52	132.11	123.70
22	BA	382	A	C5-C6-N6	10.52	132.11	123.70
22	BA	1746	A	C5-C6-N6	10.52	132.11	123.70
22	BA	2005	A	N7-C8-N9	-10.52	108.54	113.80
22	BA	2459	A	N3-C4-C5	-10.52	119.44	126.80
1	AA	460	A	C5-C6-N6	10.51	132.11	123.70
22	BA	2094	A	C5-C6-N6	10.51	132.11	123.70
22	BA	2434	A	N7-C8-N9	-10.51	108.54	113.80
22	BA	219	A	C5-C6-N6	10.51	132.11	123.70
22	BA	443	A	N7-C8-N9	-10.51	108.54	113.80
1	AA	649	A	N7-C8-N9	-10.51	108.55	113.80
1	AA	1362	A	N7-C8-N9	-10.51	108.55	113.80
1	AA	336	A	N7-C8-N9	-10.51	108.55	113.80
22	BA	300	A	C5-C6-N6	10.51	132.10	123.70
22	BA	430	A	N7-C8-N9	-10.51	108.55	113.80
22	BA	751	A	C5-C6-N6	10.51	132.10	123.70
22	BA	1085	A	N7-C8-N9	-10.51	108.55	113.80
22	BA	1745	A	N7-C8-N9	-10.51	108.55	113.80
22	BA	2003	A	N3-C4-C5	-10.51	119.45	126.80
22	BA	2868	A	N3-C4-C5	-10.51	119.45	126.80
1	AA	116	A	N3-C4-C5	-10.50	119.45	126.80
1	AA	1254	A	N7-C8-N9	-10.50	108.55	113.80
1	AA	1483	A	C5-C6-N6	10.50	132.10	123.70
22	BA	1548	A	C5-C6-N6	10.50	132.10	123.70
22	BA	2560	A	N7-C8-N9	-10.50	108.55	113.80
22	BA	2311	A	N7-C8-N9	-10.50	108.55	113.80
22	BA	2665	A	C5-C6-N6	10.50	132.10	123.70
22	BA	2711	A	C5-C6-N6	10.50	132.10	123.70
22	BA	2809	A	C5-C6-N6	10.50	132.10	123.70
1	AA	77	A	N3-C4-C5	-10.50	119.45	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1142	A	C5-C6-N6	10.50	132.10	123.70
1	AA	900	A	N7-C8-N9	-10.49	108.55	113.80
22	BA	2850	A	N3-C4-C5	-10.49	119.45	126.80
1	AA	498	A	C5-C6-N1	10.49	122.95	117.70
1	AA	831	A	C5-C6-N6	10.49	132.09	123.70
1	AA	1275	A	C5-C6-N6	10.49	132.09	123.70
22	BA	1014	A	C5-C6-N6	10.49	132.09	123.70
22	BA	1169	A	C5-C6-N6	10.49	132.09	123.70
22	BA	2327	A	N3-C4-C5	-10.49	119.45	126.80
22	BA	2634	A	N3-C4-C5	-10.49	119.46	126.80
1	AA	907	A	N7-C8-N9	-10.49	108.56	113.80
22	BA	2614	A	C5-C6-N6	10.49	132.09	123.70
22	BA	480	A	N3-C4-C5	-10.49	119.46	126.80
1	AA	907	A	C5-C6-N6	10.48	132.09	123.70
22	BA	457	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	2469	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	53	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	119	A	N7-C8-N9	-10.48	108.56	113.80
1	AA	560	A	C5-C6-N6	10.48	132.08	123.70
1	AA	1102	A	C5-C6-N6	10.48	132.08	123.70
22	BA	532	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	984	A	N3-C4-C5	-10.48	119.47	126.80
22	BA	1597	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	1927	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	2077	A	N3-C4-C5	-10.48	119.47	126.80
1	AA	1465	A	N7-C8-N9	-10.47	108.56	113.80
22	BA	14	A	C5-C6-N6	10.47	132.08	123.70
22	BA	149	A	N3-C4-C5	-10.47	119.47	126.80
22	BA	480	A	C5-C6-N6	10.47	132.08	123.70
22	BA	508	A	N7-C8-N9	-10.47	108.56	113.80
22	BA	1938	A	N7-C8-N9	-10.47	108.56	113.80
22	BA	2003	A	N7-C8-N9	-10.47	108.56	113.80
22	BA	654	A	C5-C6-N6	10.47	132.08	123.70
1	AA	630	A	N7-C8-N9	-10.47	108.57	113.80
22	BA	1508	A	C5-C6-N6	10.47	132.07	123.70
22	BA	2058	A	C5-C6-N6	10.47	132.07	123.70
22	BA	2635	A	C5-C6-N6	10.47	132.07	123.70
1	AA	977	A	N3-C4-C5	-10.46	119.47	126.80
22	BA	2369	A	N7-C8-N9	-10.47	108.57	113.80
1	AA	1152	A	C5-C6-N6	10.46	132.07	123.70
22	BA	505	A	C5-C6-N6	10.46	132.07	123.70
22	BA	1528	A	N3-C4-C5	-10.47	119.47	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2199	A	N3-C4-C5	-10.47	119.47	126.80
22	BA	1551	A	N7-C8-N9	-10.46	108.57	113.80
1	AA	139	A	C5-C6-N6	10.46	132.07	123.70
1	AA	174	A	N7-C8-N9	-10.46	108.57	113.80
1	AA	303	A	N7-C8-N9	-10.46	108.57	113.80
1	AA	373	A	C5-C6-N6	10.46	132.07	123.70
22	BA	1392	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	2183	A	C5-C6-N6	10.46	132.07	123.70
23	BB	115	A	N7-C8-N9	-10.46	108.57	113.80
1	AA	535	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	715	A	C5-C6-N6	10.46	132.07	123.70
22	BA	752	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	1469	A	C5-C6-N6	10.46	132.07	123.70
22	BA	1757	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	2426	A	C5-C6-N6	10.46	132.06	123.70
23	BB	101	A	C4-C5-C6	10.46	122.23	117.00
1	AA	155	A	N7-C8-N9	-10.46	108.57	113.80
1	AA	1035	A	N3-C4-C5	-10.46	119.48	126.80
1	AA	1238	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	1735	A	C5-C6-N6	10.46	132.06	123.70
22	BA	2184	A	C5-C6-N6	10.46	132.06	123.70
22	BA	1156	A	N7-C8-N9	-10.45	108.57	113.80
22	BA	1641	A	N3-C4-C5	-10.45	119.48	126.80
1	AA	743	A	N3-C4-C5	-10.45	119.48	126.80
22	BA	1877	A	N7-C8-N9	-10.45	108.58	113.80
22	BA	2758	A	N7-C8-N9	-10.45	108.58	113.80
1	AA	1012	A	N3-C4-C5	-10.45	119.48	126.80
22	BA	272	A	N7-C8-N9	-10.45	108.58	113.80
22	BA	1304	A	C5-C6-N6	10.45	132.06	123.70
22	BA	1913	A	C5-C6-N6	10.45	132.06	123.70
1	AA	10	A	N7-C8-N9	-10.45	108.58	113.80
1	AA	382	A	N3-C4-C5	-10.45	119.49	126.80
1	AA	579	A	N3-C4-C5	-10.45	119.49	126.80
1	AA	908	A	N7-C8-N9	-10.45	108.58	113.80
22	BA	1616	A	N7-C8-N9	-10.45	108.58	113.80
23	BB	109	A	N7-C8-N9	-10.45	108.58	113.80
22	BA	460	A	C5-C6-N6	10.44	132.06	123.70
1	AA	1044	A	N7-C8-N9	-10.44	108.58	113.80
1	AA	694	A	N7-C8-N9	-10.44	108.58	113.80
1	AA	1318	A	N7-C8-N9	-10.44	108.58	113.80
1	AA	1396	A	N7-C8-N9	-10.44	108.58	113.80
22	BA	722	A	N7-C8-N9	-10.44	108.58	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	964	A	N3-C4-C5	-10.44	119.50	126.80
1	AA	1363	A	N3-C4-C5	-10.44	119.49	126.80
22	BA	1127	A	N7-C8-N9	-10.43	108.58	113.80
22	BA	1373	A	N3-C4-C5	-10.43	119.50	126.80
1	AA	1229	A	C5-C6-N6	10.43	132.05	123.70
22	BA	735	A	N7-C8-N9	-10.43	108.58	113.80
22	BA	1247	A	C5-C6-N6	10.43	132.05	123.70
22	BA	1677	A	N7-C8-N9	-10.43	108.58	113.80
1	AA	1046	A	N7-C8-N9	-10.43	108.58	113.80
1	AA	478	A	N7-C8-N9	-10.43	108.59	113.80
22	BA	2634	A	N7-C8-N9	-10.43	108.59	113.80
1	AA	1429	A	N7-C8-N9	-10.43	108.59	113.80
1	AA	315	A	C5-C6-N6	10.42	132.04	123.70
1	AA	918	A	N7-C8-N9	-10.42	108.59	113.80
1	AA	1408	A	N7-C8-N9	-10.42	108.59	113.80
22	BA	471	A	C5-C6-N6	10.42	132.04	123.70
22	BA	983	A	C5-C6-N6	10.42	132.04	123.70
1	AA	1413	A	N7-C8-N9	-10.42	108.59	113.80
22	BA	1269	A	N3-C4-C5	-10.42	119.51	126.80
1	AA	1468	A	N7-C8-N9	-10.42	108.59	113.80
22	BA	255	A	N3-C4-C5	-10.42	119.51	126.80
22	BA	632	A	C5-C6-N6	10.42	132.03	123.70
22	BA	1549	A	N7-C8-N9	-10.42	108.59	113.80
1	AA	749	A	N7-C8-N9	-10.41	108.59	113.80
1	AA	831	A	N7-C8-N9	-10.41	108.59	113.80
22	BA	753	A	C5-C6-N6	10.41	132.03	123.70
22	BA	1367	A	N3-C4-C5	-10.41	119.51	126.80
1	AA	1012	A	N7-C8-N9	-10.41	108.59	113.80
1	AA	1251	A	N7-C8-N9	-10.41	108.59	113.80
22	BA	1966	A	C5-C6-N6	10.41	132.03	123.70
1	AA	1167	A	C5-C6-N6	10.41	132.03	123.70
22	BA	1593	A	C5-C6-N6	10.41	132.03	123.70
22	BA	972	A	N3-C4-C5	-10.41	119.51	126.80
1	AA	382	A	C5-C6-N6	10.41	132.03	123.70
1	AA	393	A	N7-C8-N9	-10.41	108.60	113.80
1	AA	3	A	N7-C8-N9	-10.41	108.60	113.80
1	AA	716	A	C5-C6-N6	10.41	132.03	123.70
1	AA	1055	A	N7-C8-N9	-10.41	108.60	113.80
1	AA	1274	A	C5-C6-N6	10.41	132.03	123.70
22	BA	330	A	N7-C8-N9	-10.41	108.60	113.80
22	BA	1780	A	N7-C8-N9	-10.41	108.60	113.80
1	AA	546	A	N7-C8-N9	-10.40	108.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	579	A	C5-C6-N6	10.40	132.02	123.70
1	AA	1324	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	1672	A	N3-C4-C5	-10.40	119.52	126.80
1	AA	16	A	N7-C8-N9	-10.40	108.60	113.80
22	BA	781	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	2577	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	2765	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	2225	A	N7-C8-N9	-10.40	108.60	113.80
55	B8	58	A	C5-C6-N6	10.40	132.02	123.70
22	BA	1711	A	N7-C8-N9	-10.40	108.60	113.80
22	BA	190	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	2639	A	N7-C8-N9	-10.40	108.60	113.80
22	BA	981	A	N7-C8-N9	-10.40	108.60	113.80
22	BA	2516	A	N3-C4-C5	-10.40	119.52	126.80
1	AA	648	A	N7-C8-N9	-10.39	108.60	113.80
1	AA	673	A	C5-C6-N6	10.39	132.01	123.70
1	AA	179	A	N7-C8-N9	-10.39	108.61	113.80
1	AA	300	A	C4-C5-C6	10.39	122.20	117.00
22	BA	1403	A	N7-C8-N9	-10.39	108.61	113.80
22	BA	1713	A	N7-C8-N9	-10.39	108.61	113.80
22	BA	2211	A	N7-C8-N9	-10.39	108.61	113.80
23	BB	15	A	C5-C6-N6	10.39	132.01	123.70
1	AA	303	A	C5-C6-N6	10.39	132.01	123.70
22	BA	2829	A	N7-C8-N9	-10.38	108.61	113.80
23	BB	57	A	N3-C4-C5	-10.38	119.53	126.80
55	B8	51	A	C5-C6-N6	10.38	132.01	123.70
1	AA	574	A	N7-C8-N9	-10.38	108.61	113.80
22	BA	928	A	N3-C4-C5	-10.38	119.53	126.80
22	BA	2826	A	N3-C4-C5	-10.38	119.53	126.80
1	AA	1434	A	N7-C8-N9	-10.38	108.61	113.80
22	BA	2899	A	N7-C8-N9	-10.38	108.61	113.80
22	BA	218	A	C5-C6-N6	10.38	132.00	123.70
22	BA	348	A	C5-C6-N6	10.38	132.00	123.70
22	BA	2564	A	C5-C6-N6	10.38	132.00	123.70
1	AA	1152	A	N3-C4-C5	-10.38	119.54	126.80
1	AA	1360	A	N7-C8-N9	-10.38	108.61	113.80
22	BA	1020	A	N7-C8-N9	-10.38	108.61	113.80
1	AA	19	A	C5-C6-N6	10.37	132.00	123.70
1	AA	1155	A	C5-C6-N6	10.37	132.00	123.70
22	BA	262	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	627	A	N7-C8-N9	-10.37	108.61	113.80
22	BA	1570	A	N7-C8-N9	-10.37	108.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	236	A	N7-C8-N9	-10.37	108.62	113.80
1	AA	1441	A	C5-C6-N6	10.37	132.00	123.70
22	BA	44	A	N3-C4-C5	-10.37	119.54	126.80
1	AA	441	A	N7-C8-N9	-10.37	108.62	113.80
22	BA	155	A	N7-C8-N9	-10.37	108.62	113.80
1	AA	1256	A	C5-C6-N6	10.37	131.99	123.70
22	BA	727	A	N7-C8-N9	-10.37	108.62	113.80
22	BA	1810	A	C4-C5-C6	10.37	122.18	117.00
22	BA	2734	A	N7-C8-N9	-10.37	108.62	113.80
22	BA	920	A	N7-C8-N9	-10.36	108.62	113.80
22	BA	1214	A	N3-C4-C5	-10.36	119.55	126.80
1	AA	282	A	N7-C8-N9	-10.36	108.62	113.80
22	BA	439	A	N3-C4-C5	-10.36	119.55	126.80
22	BA	761	A	N3-C4-C5	-10.36	119.55	126.80
22	BA	2205	A	C5-C6-N6	10.36	131.99	123.70
22	BA	2886	A	C5-C6-N6	10.36	131.99	123.70
22	BA	1749	A	N7-C8-N9	-10.36	108.62	113.80
1	AA	298	A	C5-C6-N6	10.36	131.99	123.70
1	AA	356	A	N7-C8-N9	-10.36	108.62	113.80
1	AA	389	A	C5-C6-N6	10.36	131.99	123.70
22	BA	844	A	C5-C6-N6	10.36	131.99	123.70
22	BA	1722	A	N3-C4-C5	-10.36	119.55	126.80
22	BA	2090	A	N3-C4-C5	-10.36	119.55	126.80
55	B8	69	A	C5-C6-N6	10.36	131.99	123.70
1	AA	325	A	N7-C8-N9	-10.35	108.62	113.80
1	AA	728	A	N7-C8-N9	-10.35	108.62	113.80
22	BA	439	A	N7-C8-N9	-10.35	108.62	113.80
22	BA	2660	A	N7-C8-N9	-10.35	108.62	113.80
22	BA	825	A	N3-C4-C5	-10.35	119.55	126.80
22	BA	2094	A	N7-C8-N9	-10.35	108.62	113.80
1	AA	1368	A	N7-C8-N9	-10.35	108.63	113.80
22	BA	1098	A	N7-C8-N9	-10.35	108.63	113.80
1	AA	1157	A	N7-C8-N9	-10.35	108.63	113.80
22	BA	2851	A	C5-C6-N6	10.35	131.98	123.70
23	BB	34	A	N7-C8-N9	-10.35	108.63	113.80
1	AA	665	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	730	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	2097	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	2868	A	C5-C6-N6	10.34	131.97	123.70
22	BA	146	A	C5-C6-N6	10.34	131.97	123.70
1	AA	71	A	N7-C8-N9	-10.34	108.63	113.80
1	AA	435	A	N7-C8-N9	-10.34	108.63	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1591	A	N7-C8-N9	-10.34	108.63	113.80
1	AA	389	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	675	A	N7-C8-N9	-10.34	108.63	113.80
1	AA	1398	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	2297	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	354	A	C5-C6-N6	10.34	131.97	123.70
22	BA	947	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	2317	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	2635	A	N3-C4-C5	-10.34	119.56	126.80
1	AA	223	A	N3-C4-C5	-10.33	119.57	126.80
1	AA	1170	A	N3-C4-C5	-10.33	119.57	126.80
22	BA	1431	A	N3-C4-C5	-10.33	119.57	126.80
22	BA	2268	A	N7-C8-N9	-10.33	108.63	113.80
22	BA	2879	A	N3-C4-C5	-10.33	119.57	126.80
55	B8	6	A	C5-C6-N6	10.33	131.97	123.70
1	AA	199	A	N3-C4-C5	-10.33	119.57	126.80
1	AA	1110	A	N7-C8-N9	-10.33	108.64	113.80
22	BA	1689	A	N7-C8-N9	-10.33	108.64	113.80
22	BA	2826	A	N7-C8-N9	-10.33	108.64	113.80
1	AA	199	A	N7-C8-N9	-10.33	108.64	113.80
1	AA	781	A	N7-C8-N9	-10.33	108.64	113.80
22	BA	877	A	N7-C8-N9	-10.33	108.64	113.80
22	BA	1048	A	N7-C8-N9	-10.33	108.64	113.80
23	BB	57	A	N7-C8-N9	-10.33	108.64	113.80
1	AA	415	A	N3-C4-C5	-10.32	119.57	126.80
55	B8	76	A	C5-C6-N6	10.32	131.96	123.70
1	AA	246	A	C5-C6-N6	10.32	131.96	123.70
22	BA	332	A	N7-C8-N9	-10.32	108.64	113.80
1	AA	487	A	N3-C4-C5	-10.32	119.58	126.80
1	AA	729	A	C5-C6-N6	10.32	131.96	123.70
22	BA	941	A	N3-C4-C5	-10.32	119.58	126.80
1	AA	263	A	N7-C8-N9	-10.32	108.64	113.80
1	AA	865	A	N3-C4-C5	-10.32	119.58	126.80
1	AA	946	A	N3-C4-C5	-10.32	119.58	126.80
1	AA	1130	A	N7-C8-N9	-10.32	108.64	113.80
22	BA	1528	A	N7-C8-N9	-10.32	108.64	113.80
22	BA	1571	A	N3-C4-C5	-10.32	119.58	126.80
22	BA	2887	A	N7-C8-N9	-10.32	108.64	113.80
1	AA	520	A	N7-C8-N9	-10.31	108.64	113.80
22	BA	1654	A	C5-C6-N6	10.31	131.95	123.70
22	BA	1952	A	C5-C6-N6	10.31	131.95	123.70
1	AA	456	A	C5-C6-N6	10.31	131.95	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1802	A	N3-C4-C5	-10.31	119.58	126.80
1	AA	759	A	N7-C8-N9	-10.31	108.65	113.80
1	AA	1363	A	N7-C8-N9	-10.31	108.65	113.80
1	AA	595	A	N7-C8-N9	-10.31	108.65	113.80
22	BA	668	A	C5-C6-N6	10.31	131.95	123.70
1	AA	1216	A	C5-C6-N6	10.31	131.94	123.70
22	BA	1549	A	N3-C4-C5	-10.31	119.59	126.80
1	AA	635	A	C5-C6-N6	10.30	131.94	123.70
1	AA	1429	A	C5-C6-N6	10.30	131.94	123.70
22	BA	1080	A	N7-C8-N9	-10.30	108.65	113.80
23	BB	78	A	N7-C8-N9	-10.30	108.65	113.80
22	BA	538	A	N7-C8-N9	-10.30	108.65	113.80
22	BA	943	A	N3-C4-C5	-10.30	119.59	126.80
1	AA	807	A	N7-C8-N9	-10.30	108.65	113.80
22	BA	1981	A	N7-C8-N9	-10.30	108.65	113.80
1	AA	573	A	N7-C8-N9	-10.30	108.65	113.80
22	BA	460	A	N7-C8-N9	-10.30	108.65	113.80
1	AA	648	A	C5-C6-N6	10.30	131.94	123.70
1	AA	101	A	N7-C8-N9	-10.29	108.65	113.80
1	AA	250	A	N7-C8-N9	-10.29	108.65	113.80
22	BA	401	A	N3-C4-C5	-10.29	119.59	126.80
1	AA	101	A	C5-C6-N6	10.29	131.93	123.70
1	AA	167	A	C5-C6-N6	10.29	131.93	123.70
22	BA	94	A	N3-C4-C5	-10.29	119.59	126.80
22	BA	1586	A	N3-C4-C5	-10.29	119.60	126.80
22	BA	2327	A	C5-C6-N6	10.29	131.93	123.70
1	AA	1252	A	N3-C4-C5	-10.29	119.60	126.80
1	AA	72	A	N7-C8-N9	-10.29	108.66	113.80
1	AA	959	A	N7-C8-N9	-10.29	108.66	113.80
22	BA	182	A	C5-C6-N6	10.29	131.93	123.70
22	BA	221	A	N7-C8-N9	-10.29	108.66	113.80
22	BA	2108	A	C5-C6-N6	10.29	131.93	123.70
1	AA	373	A	N7-C8-N9	-10.28	108.66	113.80
1	AA	946	A	N7-C8-N9	-10.28	108.66	113.80
22	BA	661	A	C5-C6-N6	10.29	131.93	123.70
1	AA	1042	A	N7-C8-N9	-10.28	108.66	113.80
1	AA	1179	A	N7-C8-N9	-10.28	108.66	113.80
1	AA	1429	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	1918	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	2740	A	N7-C8-N9	-10.28	108.66	113.80
22	BA	2247	A	C5-C6-N6	10.28	131.92	123.70
1	AA	994	A	N3-C4-C5	-10.28	119.61	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1580	A	N7-C8-N9	-10.28	108.66	113.80
22	BA	2322	A	N7-C8-N9	-10.28	108.66	113.80
1	AA	510	A	N7-C8-N9	-10.28	108.66	113.80
1	AA	892	A	N3-C4-C5	-10.28	119.61	126.80
1	AA	1287	A	N7-C8-N9	-10.28	108.66	113.80
22	BA	735	A	N3-C4-C5	-10.28	119.61	126.80
22	BA	750	A	C5-C6-N6	10.28	131.92	123.70
22	BA	1111	A	C5-C6-N6	10.28	131.92	123.70
22	BA	1262	A	N3-C4-C5	-10.28	119.61	126.80
23	BB	94	A	C5-C6-N6	10.28	131.92	123.70
1	AA	1236	A	C5-C6-N6	10.27	131.92	123.70
1	AA	1350	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	1848	A	N7-C8-N9	-10.27	108.66	113.80
22	BA	2212	A	N7-C8-N9	-10.27	108.66	113.80
22	BA	2635	A	N7-C8-N9	-10.27	108.66	113.80
1	AA	19	A	N7-C8-N9	-10.27	108.67	113.80
22	BA	231	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	412	A	C5-C6-N6	10.27	131.92	123.70
22	BA	556	A	C5-C6-N6	10.27	131.92	123.70
22	BA	1711	A	C5-C6-N6	10.27	131.92	123.70
22	BA	582	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	756	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	2634	A	C5-C6-N6	10.27	131.92	123.70
1	AA	1360	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	384	A	N7-C8-N9	-10.27	108.67	113.80
22	BA	2900	A	N3-C4-C5	-10.27	119.61	126.80
1	AA	363	A	N7-C8-N9	-10.27	108.67	113.80
22	BA	176	A	N3-C4-C5	-10.27	119.61	126.80
1	AA	608	A	N7-C8-N9	-10.27	108.67	113.80
22	BA	825	A	N7-C8-N9	-10.27	108.67	113.80
22	BA	1353	A	N9-C4-C5	10.27	109.91	105.80
1	AA	919	A	N7-C8-N9	-10.26	108.67	113.80
1	AA	1035	A	N7-C8-N9	-10.26	108.67	113.80
1	AA	1280	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	103	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	126	A	C5-C6-N6	10.26	131.91	123.70
22	BA	1336	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	2019	A	N3-C4-C5	-10.26	119.61	126.80
1	AA	161	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	1749	A	N3-C4-C5	-10.26	119.62	126.80
1	AA	466	A	N3-C4-C5	-10.26	119.62	126.80
1	AA	532	A	N7-C8-N9	-10.26	108.67	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1274	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	1327	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	794	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	1532	A	C5-C6-N6	10.26	131.91	123.70
22	BA	2205	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	1754	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	2497	A	N3-C4-C5	-10.26	119.62	126.80
1	AA	119	A	N7-C8-N9	-10.26	108.67	113.80
1	AA	694	A	N3-C4-C5	-10.26	119.62	126.80
1	AA	1014	A	N7-C8-N9	-10.26	108.67	113.80
1	AA	1188	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	344	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	2518	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	2856	A	C5-C6-N6	10.26	131.91	123.70
1	AA	1333	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	1439	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	2450	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	626	A	C5-C6-N6	10.25	131.90	123.70
22	BA	482	A	C4-C5-C6	10.25	122.13	117.00
22	BA	845	A	N7-C8-N9	-10.25	108.67	113.80
22	BA	1265	A	N3-C4-C5	-10.25	119.62	126.80
22	BA	2095	A	N3-C4-C5	-10.25	119.62	126.80
22	BA	2171	A	C5-C6-N6	10.25	131.90	123.70
22	BA	2366	A	N7-C8-N9	-10.25	108.67	113.80
22	BA	2518	A	C5-C6-N6	10.25	131.90	123.70
23	BB	108	A	N7-C8-N9	-10.25	108.67	113.80
22	BA	572	A	N7-C8-N9	-10.25	108.67	113.80
1	AA	1180	A	N3-C4-C5	-10.25	119.63	126.80
22	BA	575	A	C5-C6-N6	10.25	131.90	123.70
1	AA	373	A	N3-C4-C5	-10.25	119.63	126.80
22	BA	1690	A	N7-C8-N9	-10.25	108.68	113.80
1	AA	1434	A	N3-C4-C5	-10.24	119.63	126.80
22	BA	599	A	N3-C4-C5	-10.24	119.63	126.80
22	BA	1084	A	N7-C8-N9	-10.24	108.68	113.80
1	AA	98	A	N7-C8-N9	-10.24	108.68	113.80
22	BA	706	A	N7-C8-N9	-10.24	108.68	113.80
22	BA	2705	A	N3-C4-C5	-10.24	119.63	126.80
22	BA	2733	A	N7-C8-N9	-10.24	108.68	113.80
1	AA	815	A	N7-C8-N9	-10.23	108.68	113.80
22	BA	472	A	C5-C6-N6	10.23	131.89	123.70
22	BA	802	A	N7-C8-N9	-10.23	108.68	113.80
22	BA	160	A	N7-C8-N9	-10.23	108.68	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	563	A	N7-C8-N9	-10.23	108.68	113.80
22	BA	2741	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	616	A	C5-C6-N6	10.23	131.88	123.70
22	BA	1762	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	2711	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	161	A	N7-C8-N9	-10.23	108.69	113.80
1	AA	935	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	1786	A	N7-C8-N9	-10.23	108.69	113.80
22	BA	1872	A	N3-C4-C5	-10.23	119.64	126.80
1	AA	1306	A	C5-C6-N6	10.22	131.88	123.70
1	AA	1465	A	C5-C6-N6	10.22	131.88	123.70
22	BA	2352	A	N3-C4-C5	-10.22	119.64	126.80
1	AA	1219	A	N3-C4-C5	-10.22	119.64	126.80
22	BA	348	A	N3-C4-C5	-10.22	119.65	126.80
22	BA	541	A	N3-C4-C5	-10.22	119.64	126.80
22	BA	1080	A	N3-C4-C5	-10.22	119.64	126.80
23	BB	99	A	N7-C8-N9	-10.22	108.69	113.80
1	AA	228	A	C5-C6-N6	10.22	131.88	123.70
22	BA	1353	A	N3-C4-C5	-10.22	119.65	126.80
22	BA	661	A	N3-C4-C5	-10.22	119.65	126.80
22	BA	2766	A	C5-C6-N6	10.22	131.87	123.70
1	AA	270	A	N7-C8-N9	-10.21	108.69	113.80
1	AA	1092	A	N7-C8-N9	-10.21	108.69	113.80
22	BA	56	A	N7-C8-N9	-10.21	108.69	113.80
22	BA	342	A	N7-C8-N9	-10.21	108.69	113.80
22	BA	348	A	N7-C8-N9	-10.21	108.69	113.80
22	BA	371	A	N7-C8-N9	-10.21	108.69	113.80
22	BA	1129	A	N7-C8-N9	-10.21	108.69	113.80
22	BA	2358	A	N7-C8-N9	-10.21	108.69	113.80
55	B8	59	A	N3-C4-C5	-10.22	119.65	126.80
1	AA	937	A	N7-C8-N9	-10.21	108.69	113.80
1	AA	1197	A	N3-C4-C5	-10.21	119.65	126.80
1	AA	364	A	N7-C8-N9	-10.21	108.70	113.80
1	AA	607	A	N7-C8-N9	-10.21	108.70	113.80
22	BA	1477	A	C5-C6-N6	10.21	131.87	123.70
1	AA	171	A	N7-C8-N9	-10.21	108.70	113.80
1	AA	622	A	C5-C6-N6	10.20	131.86	123.70
1	AA	790	A	C5-C6-N6	10.20	131.86	123.70
22	BA	1230	A	C5-C6-N6	10.20	131.86	123.70
22	BA	1502	A	C5-C6-N6	10.20	131.86	123.70
22	BA	1803	A	C5-C6-N6	10.20	131.86	123.70
1	AA	77	A	N7-C8-N9	-10.20	108.70	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	227	A	C5-C6-N6	10.20	131.86	123.70
22	BA	2070	A	N7-C8-N9	-10.20	108.70	113.80
1	AA	19	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	6	A	C5-C6-N6	10.20	131.86	123.70
22	BA	2095	A	N7-C8-N9	-10.20	108.70	113.80
22	BA	1655	A	N7-C8-N9	-10.20	108.70	113.80
22	BA	1689	A	C5-C6-N6	10.20	131.86	123.70
22	BA	1205	A	N7-C8-N9	-10.20	108.70	113.80
1	AA	1252	A	C5-C6-N6	10.20	131.86	123.70
1	AA	1261	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	2482	A	N3-C4-C5	-10.20	119.66	126.80
1	AA	1368	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	64	A	N7-C8-N9	-10.20	108.70	113.80
22	BA	95	A	C5-C6-N6	10.20	131.86	123.70
22	BA	173	A	N7-C8-N9	-10.20	108.70	113.80
22	BA	541	A	C5-C6-N6	10.20	131.86	123.70
22	BA	603	A	C5-C6-N6	10.20	131.86	123.70
22	BA	613	A	N7-C8-N9	-10.20	108.70	113.80
22	BA	368	A	N7-C8-N9	-10.19	108.70	113.80
22	BA	507	A	C5-C6-N6	10.19	131.85	123.70
22	BA	1998	A	N7-C8-N9	-10.19	108.70	113.80
22	BA	2675	A	N7-C8-N9	-10.19	108.70	113.80
1	AA	1157	A	C5-C6-N6	10.19	131.85	123.70
22	BA	947	A	N3-C4-C5	-10.19	119.67	126.80
1	AA	1157	A	N3-C4-C5	-10.19	119.67	126.80
22	BA	1027	A	N7-C8-N9	-10.19	108.71	113.80
22	BA	127	A	N7-C8-N9	-10.19	108.71	113.80
22	BA	1938	A	C5-C6-N6	10.19	131.85	123.70
23	BB	115	A	N3-C4-C5	-10.18	119.67	126.80
1	AA	1238	A	N3-C4-C5	-10.18	119.67	126.80
1	AA	1456	A	N7-C8-N9	-10.18	108.71	113.80
22	BA	311	A	N7-C8-N9	-10.18	108.71	113.80
1	AA	10	A	C5-C6-N6	10.18	131.84	123.70
22	BA	347	A	N3-C4-C5	-10.18	119.67	126.80
1	AA	382	A	N7-C8-N9	-10.18	108.71	113.80
1	AA	1082	A	N7-C8-N9	-10.18	108.71	113.80
22	BA	1496	A	N7-C8-N9	-10.18	108.71	113.80
1	AA	994	A	N7-C8-N9	-10.18	108.71	113.80
22	BA	925	A	N3-C4-C5	-10.18	119.67	126.80
22	BA	1772	A	N3-C4-C5	-10.18	119.67	126.80
22	BA	1039	A	N7-C8-N9	-10.18	108.71	113.80
22	BA	2386	A	N7-C8-N9	-10.18	108.71	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	546	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	454	A	N7-C8-N9	-10.17	108.71	113.80
22	BA	1640	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	2020	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	2665	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	693	A	N7-C8-N9	-10.17	108.72	113.80
22	BA	2682	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	165	A	N7-C8-N9	-10.17	108.72	113.80
22	BA	1434	A	N9-C4-C5	10.17	109.87	105.80
22	BA	1739	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	2439	A	N7-C8-N9	-10.17	108.72	113.80
1	AA	431	A	N7-C8-N9	-10.16	108.72	113.80
1	AA	878	A	N7-C8-N9	-10.16	108.72	113.80
1	AA	906	A	N7-C8-N9	-10.16	108.72	113.80
22	BA	2173	A	N7-C8-N9	-10.16	108.72	113.80
1	AA	1476	A	N7-C8-N9	-10.16	108.72	113.80
1	AA	1534	A	N7-C8-N9	-10.16	108.72	113.80
22	BA	172	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	1937	A	N7-C8-N9	-10.16	108.72	113.80
22	BA	56	A	C5-C6-N6	10.16	131.83	123.70
22	BA	592	A	N7-C8-N9	-10.16	108.72	113.80
22	BA	743	A	C5-C6-N6	10.16	131.83	123.70
22	BA	2530	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	2534	A	N7-C8-N9	-10.16	108.72	113.80
1	AA	1216	A	N7-C8-N9	-10.16	108.72	113.80
22	BA	21	A	C5-C6-N6	10.16	131.83	123.70
22	BA	160	A	N3-C4-C5	-10.16	119.69	126.80
1	AA	768	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	53	A	C5-C6-N6	10.16	131.83	123.70
22	BA	592	A	C5-C6-N6	10.16	131.83	123.70
22	BA	1969	A	N7-C8-N9	-10.16	108.72	113.80
22	BA	2135	A	N7-C8-N9	-10.16	108.72	113.80
1	AA	338	A	C5-C6-N6	10.15	131.82	123.70
22	BA	863	A	N7-C8-N9	-10.15	108.72	113.80
22	BA	1590	A	C5-C6-N6	10.15	131.82	123.70
22	BA	2461	A	N7-C8-N9	-10.15	108.72	113.80
1	AA	28	A	N3-C4-C5	-10.15	119.69	126.80
1	AA	649	A	C5-C6-N6	10.15	131.82	123.70
1	AA	864	A	N3-C4-C5	-10.15	119.69	126.80
22	BA	1698	A	N7-C8-N9	-10.15	108.72	113.80
22	BA	2425	A	N7-C8-N9	-10.15	108.72	113.80
22	BA	2748	A	N7-C8-N9	-10.15	108.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	554	A	N7-C8-N9	-10.15	108.73	113.80
22	BA	63	A	N7-C8-N9	-10.15	108.72	113.80
22	BA	1794	A	N3-C4-C5	-10.15	119.70	126.80
22	BA	2317	A	N3-C4-C5	-10.15	119.70	126.80
23	BB	50	A	N7-C8-N9	-10.15	108.73	113.80
1	AA	66	A	C5-C6-N6	10.14	131.81	123.70
1	AA	814	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	64	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	255	A	C5-C6-N6	10.14	131.81	123.70
22	BA	514	A	N7-C8-N9	-10.14	108.73	113.80
22	BA	1591	A	C5-C6-N6	10.14	131.82	123.70
22	BA	2418	A	C5-C6-N6	10.14	131.81	123.70
1	AA	448	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	1801	A	N7-C8-N9	-10.14	108.73	113.80
1	AA	704	A	N7-C8-N9	-10.14	108.73	113.80
22	BA	1194	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	2882	A	N3-C4-C5	-10.14	119.70	126.80
1	AA	816	A	N7-C8-N9	-10.14	108.73	113.80
22	BA	920	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	1274	A	C5-C6-N6	10.14	131.81	123.70
22	BA	1287	A	N3-C4-C5	-10.13	119.70	126.80
22	BA	2031	A	C5-C6-N6	10.13	131.80	123.70
1	AA	602	A	C5-C6-N6	10.13	131.80	123.70
1	AA	949	A	N3-C4-C5	-10.13	119.71	126.80
22	BA	1717	A	N3-C4-C5	-10.13	119.71	126.80
22	BA	2094	A	N3-C4-C5	-10.13	119.71	126.80
1	AA	1324	A	C5-C6-N6	10.13	131.80	123.70
1	AA	192	A	N7-C8-N9	-10.13	108.74	113.80
1	AA	753	A	N7-C8-N9	-10.12	108.74	113.80
1	AA	1306	A	N3-C4-C5	-10.12	119.71	126.80
1	AA	1418	A	N7-C8-N9	-10.13	108.74	113.80
22	BA	2077	A	C5-C6-N6	10.13	131.80	123.70
22	BA	2154	A	N3-C4-C5	-10.12	119.71	126.80
1	AA	389	A	N7-C8-N9	-10.12	108.74	113.80
22	BA	677	A	N7-C8-N9	-10.12	108.74	113.80
1	AA	262	A	N7-C8-N9	-10.12	108.74	113.80
1	AA	1306	A	N7-C8-N9	-10.12	108.74	113.80
22	BA	156	A	N7-C8-N9	-10.12	108.74	113.80
22	BA	1134	A	N7-C8-N9	-10.12	108.74	113.80
22	BA	1918	A	N7-C8-N9	-10.12	108.74	113.80
1	AA	366	A	N7-C8-N9	-10.12	108.74	113.80
1	AA	706	A	N7-C8-N9	-10.12	108.74	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2425	A	N3-C4-C5	-10.12	119.72	126.80
1	AA	55	A	C5-C6-N6	10.11	131.79	123.70
1	AA	460	A	N3-C4-C5	-10.11	119.72	126.80
1	AA	1248	A	N7-C8-N9	-10.12	108.74	113.80
2	AB	205	ASP	CB-CA-C	10.11	130.63	110.40
22	BA	503	A	N3-C4-C5	-10.12	119.72	126.80
1	AA	743	A	N7-C8-N9	-10.11	108.75	113.80
22	BA	38	A	N7-C8-N9	-10.11	108.74	113.80
22	BA	94	A	N7-C8-N9	-10.11	108.74	113.80
22	BA	282	A	C5-C6-N6	10.11	131.79	123.70
1	AA	66	A	N7-C8-N9	-10.11	108.75	113.80
22	BA	207	A	N7-C8-N9	-10.11	108.75	113.80
22	BA	1569	A	N7-C8-N9	-10.11	108.75	113.80
22	BA	1932	A	N7-C8-N9	-10.11	108.75	113.80
1	AA	1	A	N3-C4-C5	-10.11	119.72	126.80
1	AA	98	A	N3-C4-C5	-10.11	119.72	126.80
1	AA	1081	A	C5-C6-N6	10.11	131.78	123.70
22	BA	1144	A	N7-C8-N9	-10.11	108.75	113.80
22	BA	118	A	C5-C6-N6	10.11	131.78	123.70
1	AA	460	A	N7-C8-N9	-10.10	108.75	113.80
1	AA	728	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	453	A	N7-C8-N9	-10.10	108.75	113.80
1	AA	149	A	N7-C8-N9	-10.10	108.75	113.80
1	AA	1176	A	C5-C6-N6	10.10	131.78	123.70
1	AA	889	A	N7-C8-N9	-10.10	108.75	113.80
1	AA	1531	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	800	A	N7-C8-N9	-10.10	108.75	113.80
22	BA	2531	A	N3-C4-C5	-10.10	119.73	126.80
23	BB	34	A	C5-C6-N6	10.10	131.78	123.70
1	AA	909	A	N7-C8-N9	-10.10	108.75	113.80
1	AA	1476	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	613	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	1246	A	N7-C8-N9	-10.10	108.75	113.80
22	BA	1637	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	2873	A	N7-C8-N9	-10.09	108.75	113.80
1	AA	983	A	N7-C8-N9	-10.09	108.76	113.80
1	AA	1180	A	N7-C8-N9	-10.09	108.75	113.80
22	BA	196	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	142	A	N3-C4-C5	-10.09	119.74	126.80
1	AA	892	A	N7-C8-N9	-10.09	108.76	113.80
22	BA	945	A	N7-C8-N9	-10.09	108.76	113.80
22	BA	1553	A	N7-C8-N9	-10.09	108.76	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1650	A	C5-C6-N6	10.09	131.77	123.70
1	AA	816	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	195	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	2872	A	N7-C8-N9	-10.08	108.76	113.80
1	AA	1004	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	118	A	N7-C8-N9	-10.08	108.76	113.80
22	BA	429	A	N7-C8-N9	-10.08	108.76	113.80
22	BA	1413	A	N7-C8-N9	-10.08	108.76	113.80
22	BA	2013	A	N7-C8-N9	-10.08	108.76	113.80
23	BB	66	A	N7-C8-N9	-10.08	108.76	113.80
22	BA	256	A	N3-C4-C5	-10.08	119.75	126.80
22	BA	2469	A	C5-C6-N6	10.08	131.76	123.70
23	BB	45	A	N3-C4-C5	-10.08	119.75	126.80
55	B8	41	A	N3-C4-C5	-10.08	119.75	126.80
22	BA	95	A	N7-C8-N9	-10.07	108.76	113.80
22	BA	1549	A	C5-C6-N6	10.07	131.76	123.70
1	AA	608	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	265	A	N7-C8-N9	-10.07	108.76	113.80
1	AA	715	A	N3-C4-C5	-10.07	119.75	126.80
1	AA	1036	A	N3-C4-C5	-10.07	119.75	126.80
1	AA	1225	A	N3-C4-C5	-10.07	119.75	126.80
1	AA	1437	A	C5-C6-N6	10.07	131.76	123.70
22	BA	1098	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	675	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	1916	A	N7-C8-N9	-10.07	108.77	113.80
22	BA	2813	A	N3-C4-C5	-10.07	119.75	126.80
1	AA	288	A	N7-C8-N9	-10.07	108.77	113.80
22	BA	590	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	1008	A	N7-C8-N9	-10.07	108.77	113.80
22	BA	233	A	C5-C6-N6	10.07	131.75	123.70
22	BA	1088	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	1098	A	C5-C6-N6	10.07	131.75	123.70
22	BA	1103	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	1794	A	C5-C6-N6	10.07	131.75	123.70
22	BA	2126	A	N7-C8-N9	-10.07	108.77	113.80
1	AA	938	A	C5-C6-N6	10.06	131.75	123.70
22	BA	182	A	N3-C4-C5	-10.06	119.75	126.80
22	BA	833	A	N3-C4-C5	-10.06	119.75	126.80
22	BA	5	A	C5-C6-N6	10.06	131.75	123.70
22	BA	241	A	N7-C8-N9	-10.06	108.77	113.80
22	BA	466	A	N3-C4-C5	-10.06	119.75	126.80
22	BA	477	A	N3-C4-C5	-10.06	119.76	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	988	A	N7-C8-N9	-10.06	108.77	113.80
22	BA	1054	A	C5-C6-N6	10.06	131.75	123.70
22	BA	1175	A	N7-C8-N9	-10.06	108.77	113.80
22	BA	1632	A	N3-C4-C5	-10.06	119.75	126.80
54	B7	9	A	N7-C8-N9	-10.06	108.77	113.80
1	AA	532	A	C5-C6-N6	10.06	131.75	123.70
1	AA	1418	A	N3-C4-C5	-10.06	119.76	126.80
22	BA	1477	A	N7-C8-N9	-10.06	108.77	113.80
55	B8	14	A	N3-C4-C5	-10.06	119.76	126.80
1	AA	435	A	N3-C4-C5	-10.06	119.76	126.80
22	BA	1095	A	N7-C8-N9	-10.06	108.77	113.80
1	AA	1081	A	N3-C4-C5	-10.06	119.76	126.80
22	BA	1640	A	C5-C6-N6	10.05	131.74	123.70
1	AA	1102	A	N3-C4-C5	-10.05	119.76	126.80
22	BA	515	A	N7-C8-N9	-10.05	108.77	113.80
22	BA	2169	A	N7-C8-N9	-10.05	108.77	113.80
22	BA	2560	A	N3-C4-C5	-10.05	119.76	126.80
1	AA	274	A	C5-C6-N6	10.05	131.74	123.70
1	AA	329	A	N3-C4-C5	-10.05	119.77	126.80
22	BA	216	A	N7-C8-N9	-10.05	108.78	113.80
1	AA	533	A	C5-C6-N6	10.05	131.74	123.70
1	AA	1465	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	1274	A	N7-C8-N9	-10.05	108.78	113.80
22	BA	1302	A	C5-C6-N6	10.05	131.74	123.70
22	BA	2366	A	N3-C4-C5	-10.04	119.77	126.80
1	AA	1261	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	1392	A	N3-C4-C5	-10.04	119.77	126.80
1	AA	1507	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	1308	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	1552	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	52	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	699	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	2097	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	2837	A	N7-C8-N9	-10.04	108.78	113.80
1	AA	81	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	750	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	1142	A	N3-C4-C5	-10.04	119.78	126.80
22	BA	1151	A	N3-C4-C5	-10.04	119.78	126.80
22	BA	1327	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	1889	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	2411	A	N3-C4-C5	-10.03	119.78	126.80
1	AA	1433	A	N7-C8-N9	-10.03	108.78	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1701	A	N7-C8-N9	-10.03	108.78	113.80
22	BA	2080	A	N7-C8-N9	-10.03	108.78	113.80
22	BA	1354	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	2273	A	N7-C8-N9	-10.03	108.79	113.80
55	B8	42	A	N3-C4-C5	-10.03	119.78	126.80
1	AA	223	A	N7-C8-N9	-10.03	108.79	113.80
22	BA	42	A	N7-C8-N9	-10.03	108.79	113.80
22	BA	320	A	N7-C8-N9	-10.03	108.79	113.80
22	BA	616	A	N3-C4-C5	-10.03	119.78	126.80
1	AA	1152	A	N7-C8-N9	-10.02	108.79	113.80
22	BA	1819	A	N7-C8-N9	-10.02	108.79	113.80
22	BA	1301	A	N3-C4-C5	-10.02	119.78	126.80
22	BA	2212	A	N3-C4-C5	-10.02	119.78	126.80
1	AA	288	A	C5-C6-N6	10.02	131.72	123.70
1	AA	466	A	N7-C8-N9	-10.02	108.79	113.80
1	AA	1363	A	C5-C6-N6	10.02	131.72	123.70
22	BA	990	A	N3-C4-C5	-10.02	119.79	126.80
22	BA	2734	A	N3-C4-C5	-10.02	119.79	126.80
22	BA	2900	A	N7-C8-N9	-10.02	108.79	113.80
22	BA	2542	A	N7-C8-N9	-10.02	108.79	113.80
1	AA	78	A	C5-C6-N6	10.02	131.71	123.70
1	AA	288	A	N3-C4-C5	-10.01	119.79	126.80
22	BA	1032	A	N7-C8-N9	-10.01	108.79	113.80
22	BA	2425	A	C5-C6-N6	10.01	131.71	123.70
1	AA	313	A	N7-C8-N9	-10.01	108.79	113.80
1	AA	630	A	C5-C6-N6	10.01	131.71	123.70
1	AA	1236	A	N7-C8-N9	-10.01	108.80	113.80
22	BA	310	A	N7-C8-N9	-10.01	108.80	113.80
22	BA	1916	A	N3-C4-C5	-10.01	119.79	126.80
22	BA	1165	A	N7-C8-N9	-10.01	108.80	113.80
22	BA	1953	A	N7-C8-N9	-10.01	108.80	113.80
22	BA	2435	A	C5-C6-N6	10.01	131.71	123.70
1	AA	816	A	C5-C6-N6	10.00	131.70	123.70
1	AA	906	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	2154	A	C5-C6-N6	10.00	131.70	123.70
22	BA	197	A	C5-C6-N6	10.00	131.70	123.70
23	BB	119	A	C5-C6-N6	10.00	131.70	123.70
1	AA	635	A	N7-C8-N9	-10.00	108.80	113.80
22	BA	226	A	N7-C8-N9	-10.00	108.80	113.80
22	BA	404	A	N7-C8-N9	-10.00	108.80	113.80
22	BA	1829	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	2868	A	N7-C8-N9	-10.00	108.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1274	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	472	A	N7-C8-N9	-9.99	108.80	113.80
1	AA	532	A	N3-C4-C5	-9.99	119.81	126.80
22	BA	6	A	N7-C8-N9	-9.99	108.80	113.80
22	BA	743	A	N7-C8-N9	-9.99	108.80	113.80
1	AA	50	A	N7-C8-N9	-9.99	108.80	113.80
1	AA	1508	A	N3-C4-C5	-9.99	119.81	126.80
22	BA	602	A	N7-C8-N9	-9.99	108.81	113.80
22	BA	980	A	C5-C6-N6	9.99	131.69	123.70
22	BA	1987	A	C5-C6-N6	9.99	131.69	123.70
22	BA	849	A	N3-C4-C5	-9.99	119.81	126.80
22	BA	1829	A	C5-C6-N6	9.98	131.69	123.70
22	BA	52	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	497	A	N7-C8-N9	-9.98	108.81	113.80
23	BB	73	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	167	A	N3-C4-C5	-9.98	119.81	126.80
1	AA	53	A	C5-C6-N6	9.98	131.68	123.70
1	AA	1428	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	1413	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	382	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	2205	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	2778	A	N7-C8-N9	-9.98	108.81	113.80
1	AA	1350	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	173	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	300	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	449	A	C5-C6-N6	9.98	131.68	123.70
22	BA	2764	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	2821	A	C5-C6-N6	9.98	131.68	123.70
22	BA	1635	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	2052	A	N7-C8-N9	-9.97	108.81	113.80
22	BA	2662	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	1722	A	C5-C6-N6	9.97	131.68	123.70
22	BA	1805	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	2088	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	766	A	N7-C8-N9	-9.97	108.81	113.80
22	BA	1889	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	461	A	N7-C8-N9	-9.97	108.81	113.80
22	BA	2278	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	2753	A	N7-C8-N9	-9.97	108.81	113.80
1	AA	907	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	103	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	1285	A	N9-C4-C5	9.97	109.79	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1553	A	N3-C4-C5	-9.96	119.82	126.80
22	BA	1815	A	C5-C6-N6	9.96	131.67	123.70
22	BA	2015	A	C5-C6-N6	9.96	131.67	123.70
1	AA	487	A	N7-C8-N9	-9.96	108.82	113.80
22	BA	10	A	N7-C8-N9	-9.96	108.82	113.80
22	BA	2241	A	N7-C8-N9	-9.96	108.82	113.80
22	BA	2726	A	N7-C8-N9	-9.96	108.82	113.80
1	AA	1254	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	1374	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	2590	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	33	A	C5-C6-N6	9.96	131.66	123.70
1	AA	687	A	N7-C8-N9	-9.96	108.82	113.80
22	BA	340	A	N7-C8-N9	-9.96	108.82	113.80
22	BA	1866	A	C5-C6-N6	9.96	131.66	123.70
22	BA	2058	A	N7-C8-N9	-9.96	108.82	113.80
23	BB	73	A	C5-C6-N6	9.96	131.66	123.70
1	AA	1176	A	N7-C8-N9	-9.95	108.82	113.80
22	BA	751	A	N3-C4-C5	-9.95	119.83	126.80
22	BA	1809	A	N7-C8-N9	-9.95	108.82	113.80
22	BA	2872	A	C4-C5-N7	-9.95	105.72	110.70
1	AA	533	A	N7-C8-N9	-9.95	108.83	113.80
1	AA	1170	A	N7-C8-N9	-9.95	108.83	113.80
22	BA	2451	A	N3-C4-C5	-9.95	119.84	126.80
22	BA	213	A	N3-C4-C5	-9.95	119.84	126.80
22	BA	1175	A	N3-C4-C5	-9.95	119.84	126.80
1	AA	320	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	2778	A	N3-C4-C5	-9.95	119.84	126.80
22	BA	1515	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	715	A	C5-C6-N6	9.94	131.65	123.70
1	AA	1102	A	N7-C8-N9	-9.94	108.83	113.80
1	AA	1349	A	N7-C8-N9	-9.94	108.83	113.80
22	BA	38	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	2071	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	155	A	C5-C6-N6	9.94	131.65	123.70
22	BA	742	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	1387	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	1676	A	N3-C4-C5	-9.94	119.85	126.80
1	AA	116	A	N7-C8-N9	-9.93	108.83	113.80
1	AA	192	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	629	A	N7-C8-N9	-9.93	108.83	113.80
1	AA	1396	A	C5-C6-N6	9.93	131.65	123.70
1	AA	1468	A	N3-C4-C5	-9.93	119.85	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1515	A	N9-C4-C5	9.93	109.77	105.80
23	BB	94	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	1637	A	N7-C8-N9	-9.93	108.83	113.80
22	BA	2856	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	1095	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	640	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	990	A	N7-C8-N9	-9.93	108.84	113.80
22	BA	2654	A	N7-C8-N9	-9.93	108.84	113.80
1	AA	59	A	N3-C4-C5	-9.92	119.85	126.80
22	BA	1469	A	N7-C8-N9	-9.92	108.84	113.80
22	BA	453	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	1143	A	N3-C4-C5	-9.92	119.85	126.80
1	AA	1288	A	N7-C8-N9	-9.92	108.84	113.80
22	BA	492	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	1264	A	N7-C8-N9	-9.92	108.84	113.80
1	AA	635	A	N3-C4-C5	-9.92	119.86	126.80
1	AA	1093	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	917	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	1354	A	C5-C6-N6	9.92	131.63	123.70
22	BA	2037	A	C5-C6-N6	9.92	131.63	123.70
22	BA	2340	A	N3-C4-C5	-9.92	119.86	126.80
1	AA	1288	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	226	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	382	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	752	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	1365	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	1336	A	C5-C6-N6	9.91	131.63	123.70
22	BA	1551	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	32	A	N7-C8-N9	-9.91	108.84	113.80
22	BA	42	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	2757	A	C5-C6-N6	9.91	131.63	123.70
1	AA	152	A	N7-C8-N9	-9.91	108.84	113.80
1	AA	196	A	N7-C8-N9	-9.91	108.85	113.80
1	AA	814	A	N7-C8-N9	-9.91	108.84	113.80
22	BA	270	A	N7-C8-N9	-9.91	108.84	113.80
22	BA	753	A	N7-C8-N9	-9.91	108.84	113.80
22	BA	1366	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	1579	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	2476	A	N7-C8-N9	-9.91	108.84	113.80
1	AA	1093	A	N7-C8-N9	-9.91	108.85	113.80
22	BA	899	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	272	A	N3-C4-C5	-9.91	119.87	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	497	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	2191	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	2059	A	N7-C8-N9	-9.90	108.85	113.80
1	AA	718	A	N7-C8-N9	-9.90	108.85	113.80
1	AA	766	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	2900	A	C5-C6-N6	9.90	131.62	123.70
23	BB	39	A	C5-C6-N6	9.90	131.62	123.70
1	AA	579	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	844	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	1084	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	1668	A	N7-C8-N9	-9.90	108.85	113.80
1	AA	205	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	1395	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	1597	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	1876	A	C5-C6-N6	9.90	131.62	123.70
22	BA	2860	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	2453	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	1772	A	N7-C8-N9	-9.89	108.85	113.80
22	BA	2288	A	N7-C8-N9	-9.89	108.85	113.80
22	BA	2426	A	N7-C8-N9	-9.89	108.85	113.80
22	BA	28	A	N7-C8-N9	-9.89	108.86	113.80
22	BA	219	A	N3-C4-C5	-9.89	119.88	126.80
22	BA	1496	A	C5-C6-N6	9.89	131.61	123.70
22	BA	2270	A	N7-C8-N9	-9.89	108.86	113.80
22	BA	219	A	N7-C8-N9	-9.89	108.86	113.80
22	BA	2614	A	N9-C4-C5	9.89	109.76	105.80
22	BA	1001	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	1188	A	N7-C8-N9	-9.88	108.86	113.80
1	AA	1513	A	N7-C8-N9	-9.88	108.86	113.80
22	BA	621	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	2598	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	608	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	632	A	N7-C8-N9	-9.88	108.86	113.80
22	BA	743	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	272	A	C5-C6-N6	9.88	131.60	123.70
22	BA	1213	A	C5-C6-N6	9.88	131.60	123.70
22	BA	1284	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	1579	A	N7-C8-N9	-9.88	108.86	113.80
22	BA	2381	A	C5-C6-N6	9.88	131.60	123.70
22	BA	1268	A	N3-C4-C5	-9.88	119.89	126.80
22	BA	1759	A	N3-C4-C5	-9.88	119.89	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1970	A	C8-N9-C4	9.88	109.75	105.80
22	BA	2378	A	C5-C6-N6	9.88	131.60	123.70
1	AA	767	A	C5-C6-N6	9.88	131.60	123.70
1	AA	309	A	C5-C6-N6	9.87	131.60	123.70
1	AA	452	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	2013	A	C5-C6-N6	9.87	131.60	123.70
22	BA	2054	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	363	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	781	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	825	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	71	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	344	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	685	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	1073	A	N3-C4-C5	-9.87	119.89	126.80
23	BB	46	A	N7-C8-N9	-9.87	108.86	113.80
22	BA	900	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	1705	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	441	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	509	A	N7-C8-N9	-9.87	108.87	113.80
22	BA	1254	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	1746	A	N7-C8-N9	-9.87	108.87	113.80
22	BA	1901	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	2407	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	2478	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	174	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	655	A	C5-C6-N6	9.86	131.59	123.70
22	BA	1745	A	C5-C6-N6	9.87	131.59	123.70
22	BA	1848	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	1937	A	N3-C4-C5	-9.86	119.89	126.80
1	AA	1320	C	C6-N1-C2	9.86	124.25	120.30
1	AA	502	A	N7-C8-N9	-9.86	108.87	113.80
22	BA	1307	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	408	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	1054	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	1665	A	N7-C8-N9	-9.86	108.87	113.80
1	AA	448	A	N7-C8-N9	-9.86	108.87	113.80
1	AA	790	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	1055	A	C5-C6-N6	9.86	131.59	123.70
22	BA	203	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	374	A	N7-C8-N9	-9.86	108.87	113.80
1	AA	715	A	N7-C8-N9	-9.85	108.87	113.80
1	AA	977	A	N7-C8-N9	-9.85	108.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1431	A	N7-C8-N9	-9.85	108.87	113.80
22	BA	270	A	N3-C4-C5	-9.85	119.90	126.80
1	AA	1176	A	N3-C4-C5	-9.85	119.90	126.80
22	BA	2082	A	N7-C8-N9	-9.85	108.87	113.80
22	BA	2711	A	N7-C8-N9	-9.85	108.87	113.80
23	BB	59	A	C4-C5-C6	9.85	121.93	117.00
22	BA	2412	A	N7-C8-N9	-9.85	108.87	113.80
23	BB	50	A	N3-C4-C5	-9.85	119.90	126.80
1	AA	482	A	N7-C8-N9	-9.85	108.88	113.80
22	BA	199	A	N3-C4-C5	-9.85	119.91	126.80
22	BA	255	A	N7-C8-N9	-9.85	108.88	113.80
22	BA	342	A	N3-C4-C5	-9.85	119.91	126.80
22	BA	599	A	N7-C8-N9	-9.85	108.88	113.80
22	BA	1791	A	N3-C4-C5	-9.85	119.91	126.80
22	BA	2352	A	N7-C8-N9	-9.85	108.88	113.80
22	BA	2267	A	N7-C8-N9	-9.85	108.88	113.80
1	AA	270	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	1110	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	2	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	81	A	N3-C4-C5	-9.84	119.91	126.80
22	BA	1365	A	N7-C8-N9	-9.84	108.88	113.80
22	BA	1678	A	N3-C4-C5	-9.84	119.91	126.80
22	BA	1787	A	C5-C6-N6	9.84	131.57	123.70
22	BA	2589	A	N3-C4-C5	-9.84	119.91	126.80
22	BA	2799	A	N7-C8-N9	-9.84	108.88	113.80
22	BA	216	A	N3-C4-C5	-9.84	119.91	126.80
22	BA	693	A	C5-C6-N6	9.84	131.57	123.70
22	BA	2090	A	N7-C8-N9	-9.84	108.88	113.80
22	BA	706	A	N3-C4-C5	-9.84	119.92	126.80
22	BA	1439	A	N7-C8-N9	-9.84	108.88	113.80
22	BA	1744	A	N3-C4-C5	-9.84	119.92	126.80
23	BB	99	A	N3-C4-C5	-9.84	119.92	126.80
1	AA	374	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	1171	A	N7-C8-N9	-9.83	108.88	113.80
22	BA	2031	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	873	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	13	A	N7-C8-N9	-9.83	108.89	113.80
1	AA	10	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	282	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	49	A	N7-C8-N9	-9.83	108.89	113.80
22	BA	1490	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	16	A	N3-C4-C5	-9.82	119.92	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	499	A	N3-C4-C5	-9.82	119.92	126.80
23	BB	15	A	N7-C8-N9	-9.82	108.89	113.80
22	BA	447	A	N7-C8-N9	-9.82	108.89	113.80
1	AA	279	A	N7-C8-N9	-9.82	108.89	113.80
1	AA	559	A	N7-C8-N9	-9.82	108.89	113.80
1	AA	1005	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	2453	A	N7-C8-N9	-9.82	108.89	113.80
1	AA	1080	A	N7-C8-N9	-9.82	108.89	113.80
22	BA	309	A	N7-C8-N9	-9.82	108.89	113.80
22	BA	477	A	C5-C6-N6	9.82	131.56	123.70
22	BA	1900	A	N3-C4-C5	-9.82	119.93	126.80
23	BB	50	A	C5-C6-N6	9.82	131.56	123.70
1	AA	327	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	526	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	1378	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	1722	A	N7-C8-N9	-9.82	108.89	113.80
1	AA	607	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	781	A	N7-C8-N9	-9.82	108.89	113.80
1	AA	1410	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	1508	A	C5-C6-N6	9.81	131.55	123.70
22	BA	2311	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	2134	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	505	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	609	A	N7-C8-N9	-9.81	108.89	113.80
1	AA	602	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	73	A	N7-C8-N9	-9.81	108.89	113.80
1	AA	430	A	N3-C4-C5	-9.81	119.94	126.80
22	BA	983	A	N7-C8-N9	-9.81	108.90	113.80
23	BB	59	A	N7-C8-N9	-9.81	108.90	113.80
1	AA	767	A	N3-C4-C5	-9.81	119.94	126.80
1	AA	1311	A	N3-C4-C5	-9.81	119.94	126.80
1	AA	478	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	583	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	541	A	N7-C8-N9	-9.80	108.90	113.80
22	BA	749	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	833	A	C5-C6-N6	9.80	131.54	123.70
1	AA	1339	A	C5-C6-N6	9.80	131.54	123.70
22	BA	705	A	C5-C6-N6	9.80	131.54	123.70
22	BA	2657	A	N7-C8-N9	-9.80	108.90	113.80
1	AA	675	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	2009	A	C5-C6-N6	9.80	131.54	123.70
22	BA	56	A	N3-C4-C5	-9.80	119.94	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	144	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	2476	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	353	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	729	A	N7-C8-N9	-9.80	108.90	113.80
1	AA	1480	A	N7-C8-N9	-9.79	108.90	113.80
22	BA	111	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	345	A	N7-C8-N9	-9.80	108.90	113.80
22	BA	1569	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	1689	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	1960	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	2346	A	N7-C8-N9	-9.79	108.90	113.80
1	AA	681	A	C5-C6-N6	9.79	131.53	123.70
1	AA	336	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	156	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	1246	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	2097	A	C5-C6-N6	9.79	131.53	123.70
23	BB	109	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	2336	A	N7-C8-N9	-9.79	108.90	113.80
1	AA	327	A	C5-C6-N6	9.79	131.53	123.70
1	AA	790	A	N7-C8-N9	-9.79	108.91	113.80
1	AA	1055	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	1126	A	N7-C8-N9	-9.79	108.91	113.80
22	BA	2037	A	N7-C8-N9	-9.79	108.91	113.80
1	AA	1229	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	44	A	N7-C8-N9	-9.79	108.91	113.80
22	BA	933	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	979	A	N3-C4-C5	-9.78	119.95	126.80
22	BA	1403	A	C5-C6-N6	9.79	131.53	123.70
22	BA	1571	A	C5-C6-N6	9.79	131.53	123.70
22	BA	1593	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	2761	A	N7-C8-N9	-9.78	108.91	113.80
22	BA	735	A	C5-C6-N6	9.78	131.53	123.70
1	AA	802	A	N7-C8-N9	-9.78	108.91	113.80
1	AA	1375	A	N3-C4-C5	-9.78	119.95	126.80
22	BA	146	A	N3-C4-C5	-9.78	119.95	126.80
22	BA	2082	A	N3-C4-C5	-9.78	119.95	126.80
22	BA	2566	A	N7-C8-N9	-9.78	108.91	113.80
22	BA	2019	A	N7-C8-N9	-9.78	108.91	113.80
22	BA	2823	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	782	A	N7-C8-N9	-9.78	108.91	113.80
22	BA	1580	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	104	A	N3-C4-C5	-9.77	119.96	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	973	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	1872	A	C5-C6-N6	9.77	131.52	123.70
22	BA	2147	A	N7-C8-N9	-9.77	108.91	113.80
1	AA	1430	A	N7-C8-N9	-9.77	108.92	113.80
22	BA	223	A	C5-C6-N6	9.77	131.51	123.70
22	BA	699	A	N7-C8-N9	-9.77	108.92	113.80
22	BA	1276	A	N7-C8-N9	-9.77	108.92	113.80
22	BA	1665	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	2014	A	N7-C8-N9	-9.77	108.92	113.80
1	AA	1357	A	C5-C6-N6	9.77	131.51	123.70
22	BA	616	A	N7-C8-N9	-9.77	108.92	113.80
22	BA	470	A	N3-C4-C5	-9.77	119.97	126.80
22	BA	2015	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	2792	A	N3-C4-C5	-9.77	119.97	126.80
22	BA	152	A	N7-C8-N9	-9.76	108.92	113.80
22	BA	156	A	C5-C6-N6	9.76	131.51	123.70
22	BA	330	A	C5-C6-N6	9.76	131.51	123.70
22	BA	471	A	N7-C8-N9	-9.76	108.92	113.80
22	BA	1276	A	C5-C6-N6	9.76	131.51	123.70
1	AA	696	A	C5-C6-N6	9.76	131.51	123.70
22	BA	925	A	C5-C6-N6	9.76	131.51	123.70
22	BA	2184	A	N3-C4-C5	-9.76	119.97	126.80
23	BB	58	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	629	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	695	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	706	A	C5-C6-N6	9.76	131.51	123.70
22	BA	63	A	C5-C6-N6	9.76	131.50	123.70
22	BA	1509	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	749	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	670	A	N7-C8-N9	-9.75	108.92	113.80
22	BA	1603	A	C5-C6-N6	9.75	131.50	123.70
22	BA	299	A	C5-C6-N6	9.75	131.50	123.70
22	BA	756	A	N7-C8-N9	-9.75	108.92	113.80
22	BA	1384	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	747	A	N7-C8-N9	-9.75	108.93	113.80
1	AA	964	A	N7-C8-N9	-9.75	108.93	113.80
1	AA	189	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	1155	A	N7-C8-N9	-9.74	108.93	113.80
22	BA	2411	A	N7-C8-N9	-9.74	108.93	113.80
1	AA	80	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	303	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	640	A	C5-C6-N6	9.74	131.49	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1357	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	654	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	751	A	N7-C8-N9	-9.74	108.93	113.80
1	AA	937	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	199	A	N7-C8-N9	-9.74	108.93	113.80
22	BA	721	A	C5-C6-N6	9.74	131.49	123.70
22	BA	2005	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1349	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	443	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	721	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	2727	A	N7-C8-N9	-9.74	108.93	113.80
22	BA	1237	A	N7-C8-N9	-9.73	108.93	113.80
22	BA	1302	A	N3-C4-C5	-9.73	119.99	126.80
22	BA	1919	A	N7-C8-N9	-9.73	108.93	113.80
22	BA	2369	A	N3-C4-C5	-9.73	119.99	126.80
22	BA	2435	A	N7-C8-N9	-9.73	108.93	113.80
22	BA	1433	A	N7-C8-N9	-9.73	108.94	113.80
1	AA	195	A	N7-C8-N9	-9.73	108.94	113.80
22	BA	2432	A	N7-C8-N9	-9.73	108.94	113.80
1	AA	1219	A	N7-C8-N9	-9.72	108.94	113.80
22	BA	415	A	N3-C4-C5	-9.72	119.99	126.80
22	BA	1494	A	N7-C8-N9	-9.72	108.94	113.80
1	AA	72	A	N3-C4-C5	-9.72	119.99	126.80
1	AA	729	A	N3-C4-C5	-9.72	120.00	126.80
22	BA	1784	A	N3-C4-C5	-9.72	120.00	126.80
55	B8	21	A	N3-C4-C5	-9.72	119.99	126.80
1	AA	1191	A	C5-C6-N6	9.72	131.47	123.70
1	AA	1246	A	N3-C4-C5	-9.72	120.00	126.80
22	BA	975	A	N7-C8-N9	-9.72	108.94	113.80
22	BA	988	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	366	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	1021	A	C5-C6-N6	9.71	131.47	123.70
22	BA	1027	A	C5-C6-N6	9.71	131.47	123.70
22	BA	2247	A	N7-C8-N9	-9.71	108.94	113.80
1	AA	482	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	74	A	N7-C8-N9	-9.71	108.94	113.80
22	BA	144	A	C5-C6-N6	9.71	131.47	123.70
1	AA	663	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	696	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	878	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	1204	A	N7-C8-N9	-9.71	108.94	113.80
22	BA	1871	A	N7-C8-N9	-9.71	108.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2547	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	155	A	C5-C6-N6	9.71	131.47	123.70
1	AA	1155	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	911	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	1717	A	N7-C8-N9	-9.71	108.95	113.80
22	BA	2792	A	C5-C6-N6	9.71	131.47	123.70
22	BA	1877	A	N3-C4-C5	-9.71	120.01	126.80
1	AA	901	A	C5-C6-N6	9.70	131.46	123.70
23	BB	78	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	1431	A	C5-C6-N6	9.70	131.46	123.70
22	BA	165	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	2565	A	N7-C8-N9	-9.70	108.95	113.80
22	BA	1328	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	338	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	596	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	95	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	1044	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	324	A	C5-C6-N6	9.70	131.46	123.70
22	BA	508	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	2700	A	N7-C8-N9	-9.70	108.95	113.80
1	AA	1236	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	865	A	C5-C6-N6	9.69	131.45	123.70
1	AA	1000	A	C5-C6-N6	9.69	131.45	123.70
22	BA	1143	A	N7-C8-N9	-9.69	108.96	113.80
22	BA	1545	A	N3-C4-C5	-9.69	120.02	126.80
22	BA	1477	A	N3-C4-C5	-9.68	120.02	126.80
22	BA	1977	A	C5-C6-N6	9.68	131.45	123.70
1	AA	860	A	N7-C8-N9	-9.68	108.96	113.80
22	BA	197	A	N7-C8-N9	-9.68	108.96	113.80
22	BA	1262	A	N7-C8-N9	-9.68	108.96	113.80
22	BA	2227	A	N3-C4-C5	-9.68	120.02	126.80
22	BA	2564	A	N3-C4-C5	-9.68	120.03	126.80
22	BA	2736	A	N3-C4-C5	-9.68	120.02	126.80
22	BA	2469	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	1000	A	N3-C4-C5	-9.68	120.03	126.80
22	BA	1676	A	N7-C8-N9	-9.68	108.96	113.80
1	AA	151	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	1082	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	181	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	345	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	1927	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	2126	A	N3-C4-C5	-9.67	120.03	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1858	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	1105	A	C5-C6-N6	9.67	131.44	123.70
22	BA	829	A	N7-C8-N9	-9.67	108.97	113.80
22	BA	244	A	N7-C8-N9	-9.67	108.97	113.80
22	BA	477	A	N7-C8-N9	-9.67	108.97	113.80
22	BA	1413	A	C5-C6-N6	9.67	131.43	123.70
22	BA	2284	A	N7-C8-N9	-9.67	108.97	113.80
1	AA	1248	A	N3-C4-C5	-9.66	120.03	126.80
22	BA	1268	A	N7-C8-N9	-9.66	108.97	113.80
1	AA	1287	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	1496	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	2322	A	N3-C4-C5	-9.66	120.03	126.80
22	BA	1103	A	N7-C8-N9	-9.66	108.97	113.80
22	BA	1387	A	N7-C8-N9	-9.66	108.97	113.80
22	BA	2009	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	432	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	449	A	N7-C8-N9	-9.66	108.97	113.80
22	BA	460	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	722	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	1609	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	393	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	918	A	N3-C4-C5	-9.65	120.04	126.80
22	BA	1230	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	716	A	N7-C8-N9	-9.65	108.97	113.80
22	BA	689	A	C5-N7-C8	9.65	108.72	103.90
22	BA	892	A	N3-C4-C5	-9.65	120.04	126.80
22	BA	927	A	N3-C4-C5	-9.65	120.05	126.80
22	BA	2058	A	N3-C4-C5	-9.65	120.05	126.80
1	AA	53	A	N3-C4-C5	-9.65	120.05	126.80
22	BA	1434	A	N7-C8-N9	-9.65	108.97	113.80
1	AA	573	A	N3-C4-C5	-9.65	120.05	126.80
1	AA	609	A	N3-C4-C5	-9.65	120.05	126.80
22	BA	14	A	N3-C4-C5	-9.65	120.05	126.80
22	BA	402	A	N7-C8-N9	-9.65	108.98	113.80
22	BA	722	A	C5-C6-N6	9.65	131.42	123.70
22	BA	492	A	N7-C8-N9	-9.64	108.98	113.80
22	BA	1134	A	C5-C6-N6	9.64	131.41	123.70
22	BA	1155	A	C5-C6-N6	9.64	131.41	123.70
22	BA	1247	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	2810	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	1483	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	423	A	N7-C8-N9	-9.64	108.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1111	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	2015	A	N7-C8-N9	-9.64	108.98	113.80
22	BA	905	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	182	A	N7-C8-N9	-9.64	108.98	113.80
22	BA	1431	A	N7-C8-N9	-9.64	108.98	113.80
1	AA	306	A	N3-C4-C5	-9.64	120.06	126.80
1	AA	539	A	N7-C8-N9	-9.63	108.98	113.80
22	BA	402	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	936	A	C5-C6-N6	9.63	131.41	123.70
1	AA	415	A	N7-C8-N9	-9.63	108.98	113.80
1	AA	371	A	C5-C6-N6	9.63	131.40	123.70
22	BA	739	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	1230	A	N7-C8-N9	-9.63	108.98	113.80
22	BA	2088	A	C5-C6-N6	9.63	131.40	123.70
22	BA	2451	A	N9-C4-C5	9.63	109.65	105.80
1	AA	908	A	N3-C4-C5	-9.62	120.06	126.80
1	AA	1507	A	C5-C6-N6	9.62	131.40	123.70
22	BA	1544	A	N7-C8-N9	-9.62	108.99	113.80
55	B8	26	A	N3-C4-C5	-9.62	120.06	126.80
1	AA	131	A	N3-C4-C5	-9.62	120.07	126.80
1	AA	109	A	N7-C8-N9	-9.62	108.99	113.80
1	AA	1483	A	N7-C8-N9	-9.62	108.99	113.80
1	AA	199	A	C5-C6-N6	9.62	131.39	123.70
22	BA	979	A	N7-C8-N9	-9.62	108.99	113.80
22	BA	1987	A	N3-C4-C5	-9.62	120.07	126.80
22	BA	2835	A	N3-C4-C5	-9.62	120.07	126.80
1	AA	676	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	2733	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	996	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	2267	A	C5-C6-N6	9.61	131.39	123.70
1	AA	431	A	N9-C4-C5	9.61	109.64	105.80
1	AA	938	A	N7-C8-N9	-9.61	109.00	113.80
22	BA	2660	A	N3-C4-C5	-9.61	120.07	126.80
1	AA	315	A	N3-C4-C5	-9.61	120.08	126.80
1	AA	1022	A	N3-C4-C5	-9.61	120.08	126.80
22	BA	401	A	N7-C8-N9	-9.61	109.00	113.80
22	BA	2887	A	N3-C4-C5	-9.61	120.08	126.80
22	BA	2675	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	819	A	N7-C8-N9	-9.60	109.00	113.80
1	AA	149	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	364	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	2600	A	N3-C4-C5	-9.60	120.08	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2821	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	780	A	N7-C8-N9	-9.60	109.00	113.80
1	AA	784	A	C5-C6-N6	9.60	131.38	123.70
1	AA	1012	A	C5-C6-N6	9.60	131.38	123.70
22	BA	1890	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	1042	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	1938	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	2070	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	262	A	N3-C4-C5	-9.59	120.08	126.80
1	AA	270	A	C5-C6-N6	9.59	131.37	123.70
22	BA	1548	A	N3-C4-C5	-9.59	120.08	126.80
22	BA	2541	A	N3-C4-C5	-9.59	120.08	126.80
22	BA	2899	A	N3-C4-C5	-9.59	120.08	126.80
22	BA	2284	A	C5-C6-N6	9.59	131.37	123.70
1	AA	28	A	N7-C8-N9	-9.59	109.00	113.80
1	AA	155	A	N3-C4-C5	-9.59	120.09	126.80
1	AA	1105	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	152	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	556	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	2392	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	1678	A	N7-C8-N9	-9.59	109.01	113.80
22	BA	1932	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	2020	A	N7-C8-N9	-9.58	109.01	113.80
1	AA	60	A	N3-C4-C5	-9.58	120.09	126.80
22	BA	251	A	C5-C6-N6	9.58	131.37	123.70
22	BA	1057	A	N3-C4-C5	-9.58	120.09	126.80
1	AA	468	A	N3-C4-C5	-9.58	120.09	126.80
22	BA	718	A	N3-C4-C5	-9.58	120.09	126.80
22	BA	1050	A	N3-C4-C5	-9.58	120.09	126.80
22	BA	1373	A	C5-C6-N6	9.58	131.36	123.70
22	BA	2278	A	N7-C8-N9	-9.58	109.01	113.80
22	BA	2270	A	N3-C4-C5	-9.57	120.10	126.80
23	BB	53	A	N3-C4-C5	-9.57	120.10	126.80
1	AA	162	A	C4-C5-C6	9.57	121.79	117.00
1	AA	831	A	N3-C4-C5	-9.57	120.10	126.80
22	BA	1021	A	N7-C8-N9	-9.57	109.01	113.80
22	BA	1143	A	C5-C6-N6	9.57	131.36	123.70
22	BA	1635	A	N7-C8-N9	-9.57	109.01	113.80
22	BA	1669	A	C5-C6-N6	9.57	131.36	123.70
1	AA	401	C	O5'-P-OP2	-9.57	97.08	105.70
22	BA	861	A	C5-C6-N6	9.57	131.36	123.70
22	BA	1205	A	N3-C4-C5	-9.57	120.10	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2288	A	N3-C4-C5	-9.57	120.10	126.80
22	BA	2369	A	C5-C6-N6	9.57	131.36	123.70
22	BA	2386	A	C5-C6-N6	9.57	131.36	123.70
22	BA	2392	A	N7-C8-N9	-9.57	109.02	113.80
22	BA	2657	A	N3-C4-C5	-9.57	120.10	126.80
1	AA	608	A	C5-C6-N6	9.57	131.35	123.70
1	AA	1251	A	N3-C4-C5	-9.57	120.10	126.80
23	BB	94	A	N7-C8-N9	-9.57	109.02	113.80
1	AA	946	A	C5-C6-N6	9.56	131.35	123.70
22	BA	470	A	N7-C8-N9	-9.56	109.02	113.80
22	BA	63	A	N3-C4-C5	-9.56	120.11	126.80
22	BA	2378	A	N3-C4-C5	-9.56	120.11	126.80
22	BA	2340	A	C5-C6-N6	9.56	131.35	123.70
22	BA	2298	A	N3-C4-C5	-9.56	120.11	126.80
1	AA	1197	A	N7-C8-N9	-9.55	109.02	113.80
22	BA	2600	A	N7-C8-N9	-9.55	109.02	113.80
22	BA	368	A	N3-C4-C5	-9.55	120.11	126.80
22	BA	1307	A	N7-C8-N9	-9.55	109.03	113.80
22	BA	2412	A	N3-C4-C5	-9.55	120.11	126.80
22	BA	49	A	N3-C4-C5	-9.55	120.12	126.80
22	BA	1591	A	N3-C4-C5	-9.55	120.12	126.80
22	BA	2287	A	C5-C6-N6	9.55	131.34	123.70
1	AA	1275	A	N3-C4-C5	-9.55	120.12	126.80
22	BA	362	A	C5-C6-N6	9.55	131.34	123.70
22	BA	2114	A	N7-C8-N9	-9.55	109.03	113.80
22	BA	2675	A	C5-C6-N6	9.55	131.34	123.70
1	AA	1111	A	N3-C4-C5	-9.55	120.12	126.80
22	BA	412	A	N7-C8-N9	-9.54	109.03	113.80
22	BA	844	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	2176	A	N3-C4-C5	-9.54	120.12	126.80
1	AA	621	A	N7-C8-N9	-9.54	109.03	113.80
1	AA	1271	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	586	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	849	A	N7-C8-N9	-9.54	109.03	113.80
1	AA	1319	A	C8-N9-C4	9.54	109.61	105.80
1	AA	143	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	439	A	C5-C6-N6	9.54	131.33	123.70
1	AA	959	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	362	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	727	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	1027	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	2033	A	N9-C4-C5	9.53	109.61	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	263	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	602	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	1286	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	1762	A	N7-C8-N9	-9.53	109.04	113.80
22	BA	2054	A	C5-C6-N6	9.53	131.32	123.70
22	BA	1545	A	N7-C8-N9	-9.53	109.04	113.80
1	AA	1130	A	N3-C4-C5	-9.52	120.13	126.80
22	BA	1085	A	N3-C4-C5	-9.52	120.13	126.80
22	BA	101	A	C4-C5-C6	9.52	121.76	117.00
22	BA	1978	A	N3-C4-C5	-9.52	120.14	126.80
1	AA	161	A	N3-C4-C5	-9.52	120.14	126.80
23	BB	45	A	N7-C8-N9	-9.52	109.04	113.80
55	B8	66	A	N3-C4-C5	-9.52	120.14	126.80
1	AA	60	A	N7-C8-N9	-9.52	109.04	113.80
22	BA	670	A	N3-C4-C5	-9.52	120.14	126.80
22	BA	2135	A	N3-C4-C5	-9.52	120.14	126.80
1	AA	784	A	N3-C4-C5	-9.52	120.14	126.80
22	BA	472	A	N3-C4-C5	-9.52	120.14	126.80
22	BA	482	A	C5-C6-N6	9.51	131.31	123.70
22	BA	1571	A	N7-C8-N9	-9.51	109.05	113.80
1	AA	349	A	N3-C4-C5	-9.51	120.14	126.80
22	BA	19	A	C5-C6-N6	9.51	131.31	123.70
22	BA	503	A	N7-C8-N9	-9.51	109.05	113.80
22	BA	666	A	N3-C4-C5	-9.51	120.14	126.80
22	BA	2088	A	N7-C8-N9	-9.51	109.05	113.80
22	BA	432	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	1241	A	C4-C5-C6	9.50	121.75	117.00
22	BA	2439	A	N3-C4-C5	-9.50	120.15	126.80
1	AA	1014	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	2335	A	N7-C8-N9	-9.50	109.05	113.80
22	BA	1866	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	483	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	429	A	N3-C4-C5	-9.49	120.15	126.80
22	BA	1700	A	N3-C4-C5	-9.49	120.15	126.80
22	BA	2451	A	C5-C6-N6	9.49	131.30	123.70
22	BA	1679	A	N7-C8-N9	-9.49	109.05	113.80
22	BA	2287	A	N3-C4-C5	-9.49	120.16	126.80
22	BA	1698	A	N3-C4-C5	-9.49	120.16	126.80
22	BA	2090	A	C5-C6-N6	9.49	131.29	123.70
1	AA	1216	A	N3-C4-C5	-9.49	120.16	126.80
23	BB	104	A	N3-C4-C5	-9.49	120.16	126.80
22	BA	1655	A	N3-C4-C5	-9.48	120.16	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1016	A	N3-C4-C5	-9.48	120.16	126.80
1	AA	1151	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	1067	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	2435	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	213	A	C5-C6-N6	9.48	131.28	123.70
22	BA	227	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	415	A	N7-C8-N9	-9.48	109.06	113.80
22	BA	529	A	N7-C8-N9	-9.48	109.06	113.80
22	BA	789	A	N3-C4-C5	-9.48	120.16	126.80
1	AA	559	A	N3-C4-C5	-9.48	120.17	126.80
1	AA	630	A	N3-C4-C5	-9.48	120.17	126.80
1	AA	969	A	N3-C4-C5	-9.48	120.17	126.80
22	BA	633	A	N7-C8-N9	-9.48	109.06	113.80
22	BA	1284	A	N7-C8-N9	-9.48	109.06	113.80
55	B8	51	A	N3-C4-C5	-9.48	120.17	126.80
22	BA	1634	A	N3-C4-C5	-9.48	120.17	126.80
1	AA	412	A	N7-C8-N9	-9.47	109.06	113.80
22	BA	2432	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	141	G	C4-C5-N7	9.47	114.59	110.80
22	BA	574	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	676	A	N3-C4-C5	-9.47	120.17	126.80
1	AA	1534	A	N3-C4-C5	-9.47	120.17	126.80
1	AA	1151	A	C5-C6-N6	9.47	131.27	123.70
22	BA	1928	A	N7-C8-N9	-9.47	109.07	113.80
22	BA	2108	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	2169	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	1151	A	C5-C6-N6	9.46	131.27	123.70
22	BA	1773	A	N7-C8-N9	-9.46	109.07	113.80
22	BA	2542	A	N3-C4-C5	-9.46	120.17	126.80
23	BB	29	A	N3-C4-C5	-9.46	120.17	126.80
41	BT	1	MET	CB-CG-SD	-9.46	84.01	112.40
1	AA	451	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	176	A	C5-C6-N6	9.46	131.27	123.70
22	BA	299	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	1505	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	1866	A	N7-C8-N9	-9.46	109.07	113.80
22	BA	1966	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	877	A	N3-C4-C5	-9.46	120.18	126.80
1	AA	1324	A	N7-C8-N9	-9.46	109.07	113.80
22	BA	1039	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	2468	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	699	A	N9-C4-C5	9.45	109.58	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2163	A	N3-C4-C5	-9.46	120.18	126.80
1	AA	167	A	N3-C4-C5	-9.45	120.18	126.80
1	AA	1269	A	N3-C4-C5	-9.45	120.18	126.80
1	AA	702	A	N7-C8-N9	-9.45	109.08	113.80
22	BA	1366	A	N7-C8-N9	-9.45	109.07	113.80
22	BA	1384	A	N7-C8-N9	-9.45	109.07	113.80
1	AA	802	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	756	A	C5-C6-N6	9.45	131.26	123.70
22	BA	2534	A	N3-C4-C5	-9.45	120.19	126.80
1	AA	33	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	1590	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	1746	A	N3-C4-C5	-9.45	120.19	126.80
1	AA	747	A	N3-C4-C5	-9.44	120.19	126.80
1	AA	1252	A	N7-C8-N9	-9.44	109.08	113.80
22	BA	278	A	N7-C8-N9	-9.44	109.08	113.80
22	BA	626	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	1169	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	2358	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	2741	A	N9-C4-C5	9.44	109.58	105.80
1	AA	1531	A	N7-C8-N9	-9.44	109.08	113.80
1	AA	743	A	C5-C6-N6	9.44	131.25	123.70
22	BA	1090	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	2883	A	N3-C4-C5	-9.44	120.19	126.80
55	B8	38	A	C5-C6-N6	9.44	131.25	123.70
22	BA	1755	A	N3-C4-C5	-9.44	120.19	126.80
1	AA	642	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	1420	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	2346	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	705	A	C4-C5-C6	9.43	121.72	117.00
22	BA	918	A	N7-C8-N9	-9.43	109.08	113.80
22	BA	1553	A	C5-C6-N6	9.43	131.25	123.70
1	AA	595	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	1254	A	N7-C8-N9	-9.43	109.09	113.80
22	BA	1301	A	N7-C8-N9	-9.43	109.09	113.80
22	BA	1535	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	1495	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	2314	A	N3-C4-C5	-9.43	120.20	126.80
1	AA	1480	A	N3-C4-C5	-9.42	120.20	126.80
22	BA	191	A	N7-C8-N9	-9.42	109.09	113.80
22	BA	1494	A	N3-C4-C5	-9.42	120.20	126.80
22	BA	1495	A	N7-C8-N9	-9.42	109.09	113.80
22	BA	2430	A	N7-C8-N9	-9.42	109.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	452	A	C5-C6-N6	9.42	131.24	123.70
1	AA	712	A	C5-C6-N6	9.42	131.24	123.70
1	AA	1362	A	N3-C4-C5	-9.42	120.21	126.80
22	BA	354	A	N3-C4-C5	-9.42	120.21	126.80
22	BA	2281	A	N7-C8-N9	-9.42	109.09	113.80
23	BB	34	A	N3-C4-C5	-9.42	120.21	126.80
1	AA	1396	A	N3-C4-C5	-9.42	120.21	126.80
1	AA	718	A	C5-C6-N6	9.42	131.23	123.70
1	AA	51	A	N3-C4-C5	-9.41	120.21	126.80
22	BA	1321	A	N3-C4-C5	-9.41	120.21	126.80
22	BA	1502	A	N3-C4-C5	-9.41	120.21	126.80
22	BA	2726	A	N3-C4-C5	-9.41	120.21	126.80
1	AA	80	A	N7-C8-N9	-9.41	109.09	113.80
22	BA	233	A	N3-C4-C5	-9.41	120.21	126.80
1	AA	250	A	N3-C4-C5	-9.41	120.21	126.80
1	AA	649	A	N3-C4-C5	-9.41	120.21	126.80
1	AA	958	A	N3-C4-C5	-9.41	120.21	126.80
22	BA	89	A	N3-C4-C5	-9.41	120.21	126.80
22	BA	522	A	C5-C6-N6	9.41	131.23	123.70
55	B8	73	A	N3-C4-C5	-9.41	120.21	126.80
1	AA	687	A	N3-C4-C5	-9.41	120.22	126.80
22	BA	792	A	N3-C4-C5	-9.41	120.22	126.80
22	BA	866	A	N3-C4-C5	-9.41	120.22	126.80
22	BA	1872	A	N7-C8-N9	-9.41	109.10	113.80
22	BA	2433	A	C5-C6-N6	9.41	131.23	123.70
22	BA	2459	A	C5-C6-N6	9.41	131.23	123.70
9	AI	11	ARG	NE-CZ-NH1	9.40	125.00	120.30
22	BA	374	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	1014	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	1378	A	N7-C8-N9	-9.40	109.10	113.80
22	BA	1969	A	N3-C4-C5	-9.40	120.22	126.80
1	AA	1256	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	2158	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	2170	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	265	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	2183	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	454	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	928	A	N7-C8-N9	-9.40	109.10	113.80
22	BA	1876	A	N3-C4-C5	-9.39	120.22	126.80
1	AA	864	A	N7-C8-N9	-9.39	109.10	113.80
1	AA	1257	A	N3-C4-C5	-9.39	120.23	126.80
1	AA	1430	A	N3-C4-C5	-9.39	120.23	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	742	A	C5-C6-N6	9.39	131.21	123.70
22	BA	2268	A	N3-C4-C5	-9.39	120.23	126.80
1	AA	325	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	2386	A	N3-C4-C5	-9.39	120.23	126.80
1	AA	780	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	391	A	C5-C6-N6	9.39	131.21	123.70
22	BA	1285	A	N7-C8-N9	-9.38	109.11	113.80
23	BB	46	A	N3-C4-C5	-9.39	120.23	126.80
23	BB	101	A	C5-C6-N1	9.39	122.39	117.70
22	BA	1032	A	N3-C4-C5	-9.38	120.23	126.80
1	AA	1280	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	2378	A	N7-C8-N9	-9.38	109.11	113.80
22	BA	2850	A	N7-C8-N9	-9.38	109.11	113.80
1	AA	968	A	N3-C4-C5	-9.38	120.24	126.80
22	BA	203	A	N7-C8-N9	-9.38	109.11	113.80
22	BA	340	A	N3-C4-C5	-9.38	120.24	126.80
22	BA	2721	A	N7-C8-N9	-9.37	109.11	113.80
1	AA	397	A	N7-C8-N9	-9.37	109.11	113.80
1	AA	461	A	C5-C6-N6	9.37	131.20	123.70
1	AA	1146	A	N3-C4-C5	-9.37	120.24	126.80
22	BA	501	A	N3-C4-C5	-9.37	120.24	126.80
1	AA	1169	A	N3-C4-C5	-9.37	120.24	126.80
22	BA	676	A	N7-C8-N9	-9.37	109.12	113.80
1	AA	162	A	N7-C8-N9	-9.37	109.12	113.80
22	BA	74	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	1745	A	N3-C4-C5	-9.37	120.25	126.80
1	AA	914	A	N3-C4-C5	-9.36	120.25	126.80
1	AA	78	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	300	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	1126	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	1808	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	2241	A	C5-C6-N6	9.36	131.19	123.70
1	AA	663	A	C5-C6-N6	9.36	131.19	123.70
22	BA	1652	A	N7-C8-N9	-9.36	109.12	113.80
22	BA	1803	A	N3-C4-C5	-9.36	120.25	126.80
1	AA	236	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	1347	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	1773	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	1853	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	2471	A	N3-C4-C5	-9.36	120.25	126.80
23	BB	119	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	528	A	N3-C4-C5	-9.36	120.25	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2516	A	N7-C8-N9	-9.36	109.12	113.80
22	BA	666	A	C5-C6-N6	9.35	131.18	123.70
1	AA	753	A	N3-C4-C5	-9.35	120.25	126.80
1	AA	1318	A	N3-C4-C5	-9.35	120.25	126.80
1	AA	412	A	N9-C4-C5	9.35	109.54	105.80
22	BA	2059	A	N3-C4-C5	-9.35	120.25	126.80
1	AA	1398	A	N3-C4-C5	-9.35	120.26	126.80
22	BA	1134	A	N3-C4-C5	-9.35	120.26	126.80
1	AA	845	A	N3-C4-C5	-9.34	120.26	126.80
1	AA	1456	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	320	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	936	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	960	A	C4-C5-C6	9.34	121.67	117.00
22	BA	1264	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	2810	A	N7-C8-N9	-9.34	109.13	113.80
1	AA	496	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	2142	A	C5-C6-N6	9.34	131.17	123.70
22	BA	2309	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	2062	A	N3-C4-C5	-9.34	120.27	126.80
1	AA	344	A	N3-C4-C5	-9.33	120.27	126.80
1	AA	563	A	N7-C8-N9	-9.33	109.13	113.80
22	BA	1735	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	911	A	N7-C8-N9	-9.33	109.14	113.80
22	BA	959	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	574	A	N7-C8-N9	-9.33	109.14	113.80
1	AA	338	A	N7-C8-N9	-9.32	109.14	113.80
22	BA	1165	A	N3-C4-C5	-9.32	120.27	126.80
22	BA	1789	A	N7-C8-N9	-9.32	109.14	113.80
1	AA	130	A	N3-C4-C5	-9.32	120.28	126.80
1	AA	900	A	N3-C4-C5	-9.32	120.28	126.80
22	BA	1504	A	N3-C4-C5	-9.32	120.28	126.80
22	BA	1871	A	N3-C4-C5	-9.32	120.28	126.80
22	BA	2407	A	N7-C8-N9	-9.32	109.14	113.80
22	BA	2727	A	C5-C6-N6	9.32	131.16	123.70
1	AA	179	A	N3-C4-C5	-9.32	120.28	126.80
22	BA	2766	A	N7-C8-N9	-9.32	109.14	113.80
1	AA	860	A	C4-C5-C6	9.32	121.66	117.00
22	BA	1246	A	N9-C4-C5	9.32	109.53	105.80
22	BA	1634	A	N7-C8-N9	-9.32	109.14	113.80
22	BA	2426	A	N3-C4-C5	-9.32	120.28	126.80
55	B8	58	A	N3-C4-C5	-9.32	120.28	126.80
1	AA	356	A	C5-C6-N6	9.31	131.15	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	560	A	N3-C4-C5	-9.31	120.28	126.80
22	BA	2013	A	N3-C4-C5	-9.31	120.28	126.80
1	AA	3	A	N3-C4-C5	-9.31	120.28	126.80
1	AA	695	A	N7-C8-N9	-9.31	109.14	113.80
1	AA	181	A	C5-C6-N6	9.31	131.15	123.70
1	AA	716	A	N3-C4-C5	-9.31	120.28	126.80
1	AA	1508	A	N7-C8-N9	-9.31	109.14	113.80
22	BA	101	A	C5-C6-N6	9.31	131.15	123.70
22	BA	1664	A	N7-C8-N9	-9.31	109.15	113.80
22	BA	2327	A	N7-C8-N9	-9.31	109.14	113.80
22	BA	2434	A	N3-C4-C5	-9.31	120.28	126.80
1	AA	152	A	N3-C4-C5	-9.30	120.29	126.80
1	AA	807	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	1387	A	C5-C6-N6	9.31	131.15	123.70
22	BA	2014	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	2033	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	2893	A	C5-C6-N6	9.30	131.14	123.70
22	BA	430	A	N3-C4-C5	-9.30	120.29	126.80
1	AA	1507	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	2882	A	C5-N7-C8	9.30	108.55	103.90
22	BA	447	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	861	A	N7-C8-N9	-9.30	109.15	113.80
22	BA	1453	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	2037	A	N3-C4-C5	-9.30	120.29	126.80
1	AA	702	A	N3-C4-C5	-9.29	120.29	126.80
1	AA	865	A	N7-C8-N9	-9.29	109.15	113.80
22	BA	820	A	N7-C8-N9	-9.30	109.15	113.80
22	BA	1937	A	N9-C4-C5	9.30	109.52	105.80
22	BA	391	A	N3-C4-C5	-9.29	120.29	126.80
22	BA	471	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	522	A	N7-C8-N9	-9.29	109.15	113.80
22	BA	1308	A	C5-N7-C8	9.29	108.55	103.90
1	AA	768	A	N7-C8-N9	-9.29	109.16	113.80
1	AA	329	A	N7-C8-N9	-9.29	109.16	113.80
1	AA	1150	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	19	A	N3-C4-C5	-9.29	120.30	126.80
1	AA	1170	A	C4-C5-C6	9.29	121.64	117.00
22	BA	2377	A	N3-C4-C5	-9.29	120.30	126.80
1	AA	681	A	N3-C4-C5	-9.28	120.30	126.80
1	AA	1021	A	N3-C4-C5	-9.29	120.30	126.80
1	AA	171	A	N3-C4-C5	-9.28	120.30	126.80
1	AA	520	A	N3-C4-C5	-9.28	120.30	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1786	A	N3-C4-C5	-9.28	120.31	126.80
22	BA	2721	A	N3-C4-C5	-9.28	120.31	126.80
1	AA	746	A	C5-C6-N6	9.27	131.12	123.70
1	AA	1080	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	1086	A	N3-C4-C5	-9.27	120.31	126.80
1	AA	1495	U	N1-C2-O2	9.27	129.29	122.80
1	AA	1499	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	502	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	984	A	N7-C8-N9	-9.27	109.16	113.80
55	B8	69	A	N3-C4-C5	-9.27	120.31	126.80
1	AA	50	A	N3-C4-C5	-9.27	120.31	126.80
1	AA	459	A	C5-C6-N6	9.27	131.12	123.70
1	AA	746	A	N7-C8-N9	-9.27	109.17	113.80
22	BA	819	A	N7-C8-N9	-9.27	109.17	113.80
22	BA	1626	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	1711	A	N3-C4-C5	-9.27	120.31	126.80
23	BB	52	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	1028	A	N3-C4-C5	-9.26	120.31	126.80
22	BA	1214	A	N7-C8-N9	-9.26	109.17	113.80
22	BA	2632	A	N3-C4-C5	-9.26	120.32	126.80
22	BA	918	A	N3-C4-C5	-9.25	120.32	126.80
22	BA	2101	A	N3-C4-C5	-9.25	120.32	126.80
22	BA	788	A	N3-C4-C5	-9.25	120.32	126.80
1	AA	1046	A	C5-C6-N6	9.25	131.10	123.70
22	BA	1096	A	N3-C4-C5	-9.25	120.33	126.80
22	BA	2886	A	N3-C4-C5	-9.25	120.33	126.80
1	AA	1289	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	1029	A	N7-C8-N9	-9.24	109.18	113.80
22	BA	83	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	1854	A	C5-C6-N6	9.24	131.09	123.70
22	BA	2266	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	2893	A	N3-C4-C5	-9.24	120.33	126.80
23	BB	15	A	N3-C4-C5	-9.24	120.33	126.80
1	AA	819	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	195	A	N9-C4-C5	9.24	109.50	105.80
1	AA	1092	A	N3-C4-C5	-9.24	120.33	126.80
1	AA	1431	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	1978	A	C5-C6-N6	9.24	131.09	123.70
1	AA	66	A	N3-C4-C5	-9.23	120.34	126.80
22	BA	91	A	N3-C4-C5	-9.23	120.34	126.80
22	BA	1528	A	C5-C6-N6	9.23	131.09	123.70
1	AA	502	A	C5-C6-N6	9.23	131.08	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	975	A	N3-C4-C5	-9.23	120.34	126.80
22	BA	190	A	N7-C8-N9	-9.23	109.19	113.80
22	BA	1353	A	C5-N7-C8	9.23	108.51	103.90
22	BA	1641	A	C5-C6-N6	9.23	131.08	123.70
55	B8	26	A	C5-C6-N6	9.23	131.08	123.70
22	BA	621	A	N9-C4-C5	9.22	109.49	105.80
22	BA	2328	A	N3-C4-C5	-9.22	120.34	126.80
22	BA	586	A	N9-C4-C5	9.22	109.49	105.80
22	BA	909	A	C5-C6-N6	9.22	131.08	123.70
1	AA	139	A	N3-C4-C5	-9.22	120.34	126.80
22	BA	502	A	N7-C8-N9	-9.22	109.19	113.80
22	BA	1654	A	N3-C4-C5	-9.22	120.35	126.80
1	AA	129	A	N3-C4-C5	-9.22	120.35	126.80
1	AA	1167	A	N3-C4-C5	-9.22	120.35	126.80
22	BA	1809	A	N3-C4-C5	-9.22	120.35	126.80
22	BA	125	A	N3-C4-C5	-9.22	120.35	126.80
22	BA	715	A	N3-C4-C5	-9.22	120.35	126.80
22	BA	794	A	C5-C6-N6	9.22	131.07	123.70
22	BA	2147	A	N3-C4-C5	-9.22	120.35	126.80
22	BA	1508	A	N3-C4-C5	-9.22	120.35	126.80
1	AA	1413	A	N3-C4-C5	-9.21	120.35	126.80
1	AA	1179	A	N3-C4-C5	-9.21	120.35	126.80
22	BA	14	A	N7-C8-N9	-9.21	109.19	113.80
22	BA	849	A	C5-C6-N6	9.21	131.07	123.70
22	BA	371	A	N3-C4-C5	-9.21	120.35	126.80
22	BA	1713	A	N3-C4-C5	-9.21	120.35	126.80
22	BA	1077	A	N3-C4-C5	-9.21	120.35	126.80
22	BA	1189	A	N7-C8-N9	-9.21	109.19	113.80
22	BA	1901	A	N7-C8-N9	-9.21	109.19	113.80
1	AA	109	A	N3-C4-C5	-9.21	120.36	126.80
1	AA	498	A	N3-C4-N9	9.21	134.77	127.40
22	BA	1040	A	N3-C4-C5	-9.21	120.35	126.80
22	BA	1609	A	C5-C6-N6	9.21	131.07	123.70
1	AA	794	A	N3-C4-C5	-9.21	120.36	126.80
1	AA	1329	A	N3-C4-C5	-9.21	120.36	126.80
22	BA	2171	A	N3-C4-C5	-9.21	120.36	126.80
22	BA	734	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	793	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	1652	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	2679	A	C5-C6-N6	9.20	131.06	123.70
22	BA	2274	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	1552	A	N3-C4-C5	-9.20	120.36	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2333	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	2706	A	N7-C8-N9	-9.20	109.20	113.80
55	B8	38	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	526	A	N7-C8-N9	-9.19	109.20	113.80
22	BA	632	A	N3-C4-C5	-9.19	120.37	126.80
22	BA	2809	A	N3-C4-C5	-9.19	120.37	126.80
22	BA	2823	A	N7-C8-N9	-9.19	109.20	113.80
22	BA	155	A	N3-C4-C5	-9.19	120.37	126.80
22	BA	324	A	N3-C4-C5	-9.19	120.37	126.80
22	BA	2530	A	N7-C8-N9	-9.19	109.20	113.80
22	BA	505	A	N7-C8-N9	-9.19	109.21	113.80
22	BA	572	A	C5-C6-N6	9.19	131.05	123.70
22	BA	2765	A	N7-C8-N9	-9.19	109.21	113.80
1	AA	1437	A	N3-C4-C5	-9.18	120.37	126.80
22	BA	279	A	N3-C4-C5	-9.18	120.37	126.80
22	BA	470	A	C5-C6-N6	9.18	131.05	123.70
22	BA	515	A	N3-C4-C5	-9.18	120.37	126.80
22	BA	101	A	N7-C8-N9	-9.18	109.21	113.80
1	AA	197	A	N3-C4-C5	-9.18	120.38	126.80
22	BA	1787	A	N7-C8-N9	-9.18	109.21	113.80
22	BA	547	A	N3-C4-C5	-9.17	120.38	126.80
1	AA	238	A	N3-C4-C5	-9.17	120.38	126.80
1	AA	1320	C	O5'-P-OP1	-9.17	97.45	105.70
22	BA	1009	A	N3-C4-C5	-9.17	120.38	126.80
1	AA	1320	C	N3-C2-O2	9.17	128.32	121.90
1	AA	1067	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	2211	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	590	A	N7-C8-N9	-9.16	109.22	113.80
1	AA	523	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	131	A	N7-C8-N9	-9.16	109.22	113.80
22	BA	384	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	2705	A	N7-C8-N9	-9.16	109.22	113.80
22	BA	2565	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	256	A	N7-C8-N9	-9.15	109.22	113.80
22	BA	2749	A	N3-C4-C5	-9.15	120.39	126.80
1	AA	65	A	N3-C4-C5	-9.15	120.39	126.80
1	AA	414	A	N3-C4-C5	-9.15	120.39	126.80
22	BA	2418	A	N3-C4-C5	-9.15	120.39	126.80
22	BA	730	A	N7-C8-N9	-9.15	109.22	113.80
22	BA	2376	A	N3-C4-C5	-9.15	120.39	126.80
22	BA	2851	A	N3-C4-C5	-9.15	120.39	126.80
22	BA	1664	A	C4-C5-C6	9.15	121.57	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	221	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	1129	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	1821	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	1919	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	1596	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	1802	A	N7-C8-N9	-9.14	109.23	113.80
1	AA	71	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	2052	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	2381	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	2433	A	N3-C4-C5	-9.14	120.40	126.80
1	AA	1250	A	N3-C4-C5	-9.14	120.40	126.80
1	AA	190	A	N7-C8-N9	-9.14	109.23	113.80
1	AA	298	A	N3-C4-C5	-9.13	120.41	126.80
1	AA	759	A	N3-C4-C5	-9.14	120.41	126.80
1	AA	996	A	N3-C4-C5	-9.14	120.41	126.80
23	BB	59	A	N3-C4-N9	9.14	134.71	127.40
1	AA	909	A	N3-C4-C5	-9.13	120.41	126.80
1	AA	919	A	N3-C4-C5	-9.13	120.41	126.80
22	BA	1570	A	N3-C4-C5	-9.13	120.41	126.80
1	AA	74	A	N9-C4-C5	9.13	109.45	105.80
22	BA	575	A	N7-C8-N9	-9.13	109.23	113.80
22	BA	1213	A	N7-C8-N9	-9.13	109.23	113.80
22	BA	1253	A	N3-C4-C5	-9.13	120.41	126.80
22	BA	1754	A	N3-C4-C5	-9.13	120.41	126.80
1	AA	787	A	N3-C4-C5	-9.13	120.41	126.80
22	BA	1690	A	N3-C4-C5	-9.12	120.41	126.80
22	BA	1900	A	N7-C8-N9	-9.12	109.24	113.80
22	BA	2738	A	N3-C4-C5	-9.12	120.41	126.80
1	AA	44	A	N3-C4-C5	-9.12	120.41	126.80
1	AA	782	A	N3-C4-C5	-9.12	120.41	126.80
22	BA	2764	A	N3-C4-C5	-9.12	120.41	126.80
1	AA	243	A	N3-C4-C5	-9.12	120.42	126.80
22	BA	1070	A	N3-C4-C5	-9.12	120.42	126.80
22	BA	2191	A	N3-C4-C5	-9.12	120.42	126.80
22	BA	149	A	N7-C8-N9	-9.12	109.24	113.80
22	BA	1630	A	N3-C4-C5	-9.12	120.42	126.80
22	BA	2654	A	N3-C4-C5	-9.12	120.42	126.80
55	B8	66	A	C5-C6-N6	9.12	130.99	123.70
22	BA	2406	A	N3-C4-C5	-9.11	120.42	126.80
1	AA	1197	A	C5-C6-N6	9.11	130.99	123.70
1	AA	1219	A	C5-C6-N6	9.11	130.99	123.70
22	BA	1354	A	N7-C8-N9	-9.11	109.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1664	A	C5-C6-N6	9.11	130.99	123.70
22	BA	2336	A	N3-C4-C5	-9.11	120.42	126.80
1	AA	246	A	N3-C4-C5	-9.11	120.42	126.80
22	BA	2776	A	N3-C4-C5	-9.11	120.42	126.80
1	AA	1377	A	N3-C4-C5	-9.11	120.43	126.80
1	AA	554	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	633	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	2749	A	N7-C8-N9	-9.10	109.25	113.80
22	BA	2753	A	N3-C4-C5	-9.10	120.43	126.80
23	BB	66	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	1433	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	2176	A	N7-C8-N9	-9.10	109.25	113.80
22	BA	1226	A	N7-C8-N9	-9.10	109.25	113.80
22	BA	2108	A	N7-C8-N9	-9.10	109.25	113.80
22	BA	2662	A	N7-C8-N9	-9.09	109.25	113.80
22	BA	478	A	N9-C4-C5	9.09	109.44	105.80
22	BA	1848	A	N9-C4-C5	9.09	109.44	105.80
22	BA	705	A	N7-C8-N9	-9.09	109.26	113.80
22	BA	1899	A	N3-C4-C5	-9.09	120.44	126.80
1	AA	535	A	N3-C4-C5	-9.08	120.44	126.80
1	AA	648	A	N3-C4-C5	-9.08	120.44	126.80
22	BA	621	A	N7-C8-N9	-9.08	109.26	113.80
22	BA	1089	A	N3-C4-C5	-9.08	120.44	126.80
1	AA	456	A	N3-C4-C5	-9.08	120.44	126.80
22	BA	501	A	N7-C8-N9	-9.08	109.26	113.80
22	BA	310	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	2589	A	C5-N7-C8	9.07	108.44	103.90
1	AA	1204	A	N9-C4-C5	9.07	109.43	105.80
22	BA	2042	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	2813	A	N7-C8-N9	-9.07	109.26	113.80
22	BA	2060	A	N3-C4-C5	-9.07	120.45	126.80
1	AA	1408	A	N3-C4-C5	-9.06	120.46	126.80
22	BA	131	A	C4-C5-C6	9.06	121.53	117.00
22	BA	1127	A	N3-C4-C5	-9.06	120.46	126.80
22	BA	2095	A	N9-C4-C5	9.06	109.43	105.80
22	BA	2450	A	N9-C4-C5	9.06	109.42	105.80
22	BA	453	A	C5-C6-N6	9.06	130.95	123.70
22	BA	2119	A	N3-C4-C5	-9.06	120.46	126.80
22	BA	2448	A	N3-C4-C5	-9.06	120.46	126.80
22	BA	2598	A	N7-C8-N9	-9.06	109.27	113.80
1	AA	1446	A	N9-C4-C5	9.06	109.42	105.80
22	BA	800	A	N9-C4-C5	9.05	109.42	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1610	A	N3-C4-C5	-9.05	120.46	126.80
22	BA	2328	A	N7-C8-N9	-9.05	109.27	113.80
22	BA	2872	A	C5-N7-C8	9.05	108.43	103.90
1	AA	253	A	N3-C4-C5	-9.05	120.46	126.80
1	AA	1441	A	N3-C4-C5	-9.05	120.46	126.80
22	BA	1669	A	C4-C5-C6	9.05	121.53	117.00
22	BA	1953	A	N3-C4-C5	-9.05	120.47	126.80
1	AA	321	A	N3-C4-C5	-9.05	120.47	126.80
1	AA	1468	A	C5-C6-N6	9.05	130.94	123.70
22	BA	1001	A	N7-C8-N9	-9.05	109.28	113.80
22	BA	1913	A	N3-C4-C5	-9.04	120.47	126.80
1	AA	1019	A	N3-C4-C5	-9.04	120.47	126.80
1	AA	1503	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	2781	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	821	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	1383	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	582	A	C5-C6-N6	9.04	130.93	123.70
22	BA	1010	A	N7-C8-N9	-9.04	109.28	113.80
22	BA	430	A	C5-C6-N6	9.04	130.93	123.70
22	BA	739	A	N7-C8-N9	-9.04	109.28	113.80
22	BA	1936	A	N3-C4-N9	9.04	134.63	127.40
1	AA	309	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	603	A	N3-C4-C5	-9.03	120.48	126.80
23	BB	108	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	2800	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	538	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	833	A	N7-C8-N9	-9.03	109.28	113.80
22	BA	896	A	N3-C4-C5	-9.03	120.48	126.80
1	AA	974	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	6	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	529	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	947	A	C5-C6-N6	9.03	130.92	123.70
22	BA	1367	A	N7-C8-N9	-9.03	109.29	113.80
22	BA	2333	A	C5-C6-N6	9.03	130.92	123.70
1	AA	923	A	N7-C8-N9	-9.02	109.29	113.80
1	AA	1418	A	C5-C6-N6	9.02	130.92	123.70
1	AA	1433	A	N3-C4-C5	-9.02	120.48	126.80
22	BA	614	A	N3-C4-C5	-9.02	120.49	126.80
22	BA	1912	A	N3-C4-C5	-9.02	120.49	126.80
22	BA	599	A	C5-C6-N6	9.01	130.91	123.70
22	BA	1614	A	N3-C4-C5	-9.01	120.49	126.80
22	BA	2274	A	N7-C8-N9	-9.01	109.29	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2482	A	C5-C6-N6	9.01	130.91	123.70
22	BA	507	A	N3-C4-C5	-9.01	120.49	126.80
22	BA	1783	A	N7-C8-N9	-9.01	109.30	113.80
1	AA	162	A	C5-C6-N6	9.01	130.91	123.70
1	AA	777	A	N3-C4-C5	-9.01	120.50	126.80
1	AA	1394	A	N3-C4-C5	-9.01	120.50	126.80
22	BA	73	A	N3-C4-C5	-9.01	120.50	126.80
22	BA	222	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	1677	A	C5-C6-N6	9.00	130.90	123.70
22	BA	1008	A	N3-C4-C5	-8.99	120.50	126.80
22	BA	1952	A	N3-C4-C5	-8.99	120.50	126.80
22	BA	2670	A	N3-C4-C5	-8.99	120.51	126.80
22	BA	909	A	N3-C4-C5	-8.99	120.51	126.80
1	AA	815	A	N3-C4-C5	-8.99	120.51	126.80
22	BA	2883	A	C5-N7-C8	8.99	108.39	103.90
22	BA	2814	A	N3-C4-C5	-8.98	120.51	126.80
1	AA	26	A	N3-C4-C5	-8.98	120.51	126.80
1	AA	1285	A	N3-C4-C5	-8.98	120.52	126.80
1	AA	1274	A	N3-C4-C5	-8.98	120.52	126.80
22	BA	1801	A	N3-C4-C5	-8.98	120.52	126.80
1	AA	547	A	N3-C4-C5	-8.97	120.52	126.80
22	BA	309	A	N3-C4-C5	-8.97	120.52	126.80
22	BA	346	A	N3-C4-C5	-8.97	120.52	126.80
22	BA	1532	A	N3-C4-C5	-8.97	120.52	126.80
1	AA	1227	A	N3-C4-C5	-8.97	120.52	126.80
1	AA	28	A	C5-C6-N6	8.96	130.87	123.70
22	BA	1395	A	N3-C4-C5	-8.96	120.53	126.80
22	BA	2033	A	N7-C8-N9	-8.96	109.32	113.80
22	BA	2799	A	C4-C5-C6	8.96	121.48	117.00
22	BA	1705	A	C5-C6-N6	8.96	130.87	123.70
22	BA	2670	A	C5-C6-N6	8.96	130.87	123.70
22	BA	1650	A	N7-C8-N9	-8.96	109.32	113.80
55	B8	76	A	N3-C4-C5	-8.96	120.53	126.80
22	BA	2448	A	N7-C8-N9	-8.96	109.32	113.80
23	BB	39	A	N3-C4-C5	-8.96	120.53	126.80
22	BA	752	A	N9-C4-C5	8.95	109.38	105.80
22	BA	1237	A	N3-C4-C5	-8.95	120.53	126.80
22	BA	1885	A	N3-C4-C5	-8.95	120.53	126.80
1	AA	923	A	C5-C6-N6	8.95	130.86	123.70
1	AA	1204	A	N3-C4-C5	-8.95	120.54	126.80
22	BA	788	A	C5-N7-C8	8.94	108.37	103.90
22	BA	631	A	C5-C6-N6	8.94	130.85	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	120	A	N3-C4-C5	-8.94	120.54	126.80
1	AA	673	A	N7-C8-N9	-8.94	109.33	113.80
22	BA	415	A	C5-C6-N6	8.94	130.85	123.70
22	BA	231	A	C5-N7-C8	8.93	108.37	103.90
22	BA	1147	A	N3-C4-C5	-8.93	120.55	126.80
1	AA	554	A	N9-C4-C5	8.93	109.37	105.80
22	BA	781	A	N9-C4-C5	8.93	109.37	105.80
22	BA	1009	A	N7-C8-N9	-8.93	109.33	113.80
22	BA	1803	A	N7-C8-N9	-8.93	109.33	113.80
22	BA	2461	A	C5-C6-N6	8.93	130.84	123.70
22	BA	2497	A	N7-C8-N9	-8.93	109.34	113.80
22	BA	2725	A	C5-C6-N6	8.93	130.84	123.70
1	AA	704	A	N3-C4-C5	-8.92	120.56	126.80
22	BA	643	A	N3-C4-C5	-8.92	120.55	126.80
22	BA	1815	A	N3-C4-C5	-8.92	120.55	126.80
22	BA	2199	A	N7-C8-N9	-8.92	109.34	113.80
22	BA	1133	A	N7-C8-N9	-8.92	109.34	113.80
22	BA	1522	A	N3-C4-C5	-8.92	120.56	126.80
22	BA	1977	A	N3-C4-C5	-8.90	120.57	126.80
22	BA	2750	A	N3-C4-C5	-8.90	120.57	126.80
1	AA	313	A	N9-C4-C5	8.90	109.36	105.80
22	BA	118	A	N3-C4-C5	-8.90	120.57	126.80
22	BA	972	A	N7-C8-N9	-8.90	109.35	113.80
22	BA	792	A	C5-C6-N6	8.89	130.82	123.70
22	BA	2813	A	C5-C6-N6	8.89	130.82	123.70
23	BB	101	A	C5-C6-N6	8.89	130.82	123.70
1	AA	1170	A	C5-C6-N6	8.89	130.81	123.70
22	BA	282	A	N3-C4-C5	-8.89	120.58	126.80
22	BA	878	A	N3-C4-C5	-8.89	120.58	126.80
22	BA	945	A	N3-C4-C5	-8.89	120.58	126.80
22	BA	1652	A	N9-C4-C5	8.89	109.36	105.80
22	BA	2882	A	N9-C4-C5	8.89	109.36	105.80
1	AA	181	A	N3-C4-C5	-8.89	120.58	126.80
1	AA	889	A	N3-C4-C5	-8.88	120.58	126.80
22	BA	960	A	N7-C8-N9	-8.89	109.36	113.80
22	BA	152	A	C5-C6-N6	8.88	130.81	123.70
22	BA	764	A	N9-C4-C5	8.88	109.35	105.80
22	BA	960	A	C5-C6-N6	8.88	130.80	123.70
22	BA	332	A	N3-C4-C5	-8.87	120.59	126.80
23	BB	101	A	N3-C4-N9	8.87	134.50	127.40
22	BA	412	A	N3-C4-C5	-8.87	120.59	126.80
22	BA	457	A	N3-C4-C5	-8.87	120.59	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1046	A	N3-C4-C5	-8.87	120.59	126.80
22	BA	1677	A	N3-C4-C5	-8.87	120.59	126.80
22	BA	1791	A	N7-C8-N9	-8.87	109.36	113.80
22	BA	2227	A	C5-N7-C8	8.87	108.33	103.90
1	AA	520	A	N9-C4-C5	8.86	109.35	105.80
22	BA	1583	A	N3-C4-C5	-8.86	120.59	126.80
22	BA	10	A	N3-C4-C5	-8.86	120.60	126.80
22	BA	2860	A	N3-C4-C5	-8.86	120.60	126.80
22	BA	1133	A	N3-C4-C5	-8.86	120.60	126.80
22	BA	1928	A	N3-C4-C5	-8.86	120.60	126.80
22	BA	1899	A	N7-C8-N9	-8.86	109.37	113.80
1	AA	119	A	N3-C4-C5	-8.85	120.60	126.80
22	BA	53	A	N3-C4-C5	-8.85	120.60	126.80
22	BA	2577	A	N7-C8-N9	-8.85	109.37	113.80
22	BA	2764	A	N9-C4-C5	8.85	109.34	105.80
1	AA	1117	A	N3-C4-C5	-8.85	120.61	126.80
22	BA	1020	A	N3-C4-C5	-8.85	120.61	126.80
22	BA	1626	A	C5-C6-N6	8.85	130.78	123.70
22	BA	2297	A	N3-C4-C5	-8.85	120.61	126.80
22	BA	161	A	N3-C4-C5	-8.84	120.61	126.80
22	BA	428	A	N3-C4-C5	-8.84	120.61	126.80
22	BA	1701	A	N3-C4-C5	-8.84	120.61	126.80
22	BA	575	A	N3-C4-C5	-8.83	120.62	126.80
22	BA	1260	A	N7-C8-N9	-8.83	109.38	113.80
22	BA	2639	A	N3-C4-C5	-8.83	120.62	126.80
22	BA	981	A	N3-C4-C5	-8.83	120.62	126.80
22	BA	2572	A	C5-N7-C8	8.82	108.31	103.90
22	BA	1021	A	C4-C5-C6	8.82	121.41	117.00
22	BA	197	A	N3-C4-C5	-8.82	120.63	126.80
1	AA	228	A	N3-C4-C5	-8.82	120.63	126.80
1	AA	371	A	N3-C4-C5	-8.81	120.63	126.80
22	BA	1269	A	N7-C8-N9	-8.81	109.39	113.80
22	BA	627	A	N3-C4-C5	-8.81	120.63	126.80
22	BA	716	A	N3-C4-C5	-8.81	120.64	126.80
22	BA	2388	A	N3-C4-C5	-8.81	120.64	126.80
22	BA	1503	A	N3-C4-C5	-8.80	120.64	126.80
22	BA	2682	A	C5-N7-C8	8.80	108.30	103.90
1	AA	563	A	C5-C6-N6	8.80	130.74	123.70
22	BA	1783	A	N3-C4-C5	-8.80	120.64	126.80
1	AA	1492	A	N3-C4-C5	-8.79	120.64	126.80
22	BA	1304	A	N3-C4-C5	-8.79	120.64	126.80
55	B8	6	A	N3-C4-C5	-8.79	120.65	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1163	A	C5-C6-N6	8.79	130.73	123.70
22	BA	28	A	N3-C4-C5	-8.79	120.65	126.80
22	BA	204	A	N3-C4-C5	-8.78	120.65	126.80
22	BA	294	A	N3-C4-C5	-8.78	120.65	126.80
22	BA	782	A	N7-C8-N9	-8.78	109.41	113.80
22	BA	1970	A	C5-C6-N6	8.78	130.72	123.70
22	BA	513	A	C5-C6-N6	8.78	130.72	123.70
22	BA	1785	A	N7-C8-N9	-8.78	109.41	113.80
1	AA	622	A	N7-C8-N9	-8.77	109.41	113.80
1	AA	55	A	C4-C5-C6	8.76	121.38	117.00
22	BA	513	A	N7-C8-N9	-8.76	109.42	113.80
1	AA	1191	A	N7-C8-N9	-8.76	109.42	113.80
22	BA	119	A	N9-C4-C5	8.76	109.30	105.80
22	BA	800	A	N3-C4-C5	-8.76	120.67	126.80
22	BA	804	A	N3-C4-C5	-8.76	120.67	126.80
1	AA	411	A	N3-C4-C5	-8.76	120.67	126.80
22	BA	1854	A	N7-C8-N9	-8.76	109.42	113.80
1	AA	1145	A	N3-C4-C5	-8.75	120.67	126.80
22	BA	1213	A	C4-C5-C6	8.75	121.38	117.00
22	BA	1616	A	N3-C4-C5	-8.75	120.67	126.80
22	BA	631	A	N3-C4-C5	-8.75	120.68	126.80
22	BA	1528	A	C4-C5-C6	8.75	121.38	117.00
22	BA	1872	A	C4-C5-C6	8.75	121.38	117.00
1	AA	77	A	C5-C6-N6	8.75	130.70	123.70
1	AA	510	A	N3-C4-C5	-8.75	120.68	126.80
22	BA	218	A	N7-C8-N9	-8.74	109.43	113.80
22	BA	637	A	N3-C4-C5	-8.74	120.68	126.80
23	BB	59	A	C5-C6-N1	8.74	122.07	117.70
22	BA	1214	A	N9-C4-C5	8.74	109.30	105.80
1	AA	160	A	N3-C4-C5	-8.74	120.69	126.80
22	BA	677	A	C5-C6-N6	8.74	130.69	123.70
22	BA	1156	A	N3-C4-C5	-8.73	120.69	126.80
22	BA	996	A	C5-C6-N6	8.73	130.69	123.70
1	AA	498	A	C4-C5-C6	8.73	121.36	117.00
22	BA	241	A	N3-C4-C5	-8.73	120.69	126.80
22	BA	2198	A	N3-C4-C5	-8.72	120.69	126.80
54	B7	9	A	N3-C4-C5	-8.72	120.69	126.80
22	BA	2054	A	C5-N7-C8	8.72	108.26	103.90
22	BA	2388	A	C5-N7-C8	8.71	108.26	103.90
1	AA	978	A	N3-C4-C5	-8.71	120.70	126.80
1	AA	55	A	C5-N7-C8	8.70	108.25	103.90
1	AA	1299	A	C5-N7-C8	8.70	108.25	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1378	A	N9-C4-C5	8.70	109.28	105.80
1	AA	493	A	N3-C4-C5	-8.70	120.71	126.80
22	BA	609	A	N3-C4-C5	-8.70	120.71	126.80
22	BA	2577	A	N9-C4-C5	8.70	109.28	105.80
22	BA	2873	A	N3-C4-C5	-8.70	120.71	126.80
1	AA	383	A	N7-C8-N9	-8.69	109.45	113.80
1	AA	172	A	N3-C4-C5	-8.69	120.72	126.80
1	AA	766	A	N9-C4-C5	8.69	109.28	105.80
22	BA	2266	A	N7-C8-N9	-8.69	109.45	113.80
1	AA	7	A	N3-C4-C5	-8.68	120.72	126.80
22	BA	1757	A	N3-C4-C5	-8.68	120.72	126.80
1	AA	182	A	N3-C4-C5	-8.68	120.72	126.80
23	BB	101	A	N7-C8-N9	-8.68	109.46	113.80
1	AA	622	A	N3-C4-C5	-8.68	120.73	126.80
1	AA	1493	A	N3-C4-C5	-8.67	120.73	126.80
22	BA	1155	A	N3-C4-C5	-8.67	120.73	126.80
22	BA	1847	A	N9-C4-C5	8.67	109.27	105.80
22	BA	513	A	C4-C5-C6	8.67	121.33	117.00
22	BA	975	A	C5-N7-C8	8.67	108.24	103.90
22	BA	749	A	C5-N7-C8	8.66	108.23	103.90
22	BA	2530	A	N9-C4-C5	8.66	109.26	105.80
1	AA	196	A	N3-C4-C5	-8.66	120.74	126.80
22	BA	764	A	N3-C4-C5	-8.65	120.74	126.80
22	BA	1819	A	C5-N7-C8	8.65	108.23	103.90
1	AA	696	A	N7-C8-N9	-8.65	109.47	113.80
22	BA	2758	A	N3-C4-C5	-8.65	120.75	126.80
22	BA	2829	A	N3-C4-C5	-8.65	120.75	126.80
22	BA	1226	A	N3-C4-C5	-8.64	120.75	126.80
22	BA	1244	A	C5-C6-N6	8.64	130.61	123.70
22	BA	1342	A	N3-C4-C5	-8.64	120.75	126.80
1	AA	279	A	N3-C4-C5	-8.64	120.75	126.80
1	AA	1346	A	N3-C4-C5	-8.64	120.75	126.80
1	AA	860	A	N9-C4-C5	8.63	109.25	105.80
22	BA	2513	A	N7-C8-N9	-8.63	109.48	113.80
1	AA	495	A	N3-C4-C5	-8.62	120.76	126.80
22	BA	514	A	N3-C4-C5	-8.62	120.76	126.80
22	BA	1373	A	N7-C8-N9	-8.62	109.49	113.80
22	BA	1815	A	N7-C8-N9	-8.62	109.49	113.80
1	AA	195	A	N3-C4-C5	-8.62	120.76	126.80
22	BA	2042	A	C5-C6-N6	8.62	130.60	123.70
1	AA	274	A	N3-C4-C5	-8.62	120.77	126.80
1	AA	860	A	C5-N7-C8	8.62	108.21	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	915	A	N3-C4-C5	-8.62	120.77	126.80
22	BA	1470	A	N7-C8-N9	-8.62	109.49	113.80
22	BA	466	A	N7-C8-N9	-8.61	109.49	113.80
22	BA	1322	A	N3-C4-C5	-8.61	120.77	126.80
41	BT	1	MET	CB-CA-C	-8.61	93.19	110.40
22	BA	217	A	N9-C4-C5	8.60	109.24	105.80
22	BA	975	A	C4-C5-C6	8.60	121.30	117.00
1	AA	411	A	C5-C6-N6	8.59	130.57	123.70
22	BA	910	A	N3-C4-C5	-8.59	120.78	126.80
22	BA	1000	A	N9-C4-C5	8.59	109.24	105.80
22	BA	1265	A	N7-C8-N9	-8.59	109.50	113.80
22	BA	2117	A	N3-C4-C5	-8.59	120.79	126.80
22	BA	586	A	N7-C8-N9	-8.58	109.51	113.80
22	BA	1572	A	N7-C8-N9	-8.58	109.51	113.80
1	AA	913	A	N3-C4-C5	-8.57	120.80	126.80
1	AA	1213	A	N9-C4-C5	8.57	109.23	105.80
22	BA	119	A	N3-C4-C5	-8.57	120.80	126.80
1	AA	1213	A	N3-C4-C5	-8.57	120.80	126.80
22	BA	2757	A	N7-C8-N9	-8.57	109.52	113.80
22	BA	1204	A	N3-C4-C5	-8.56	120.81	126.80
22	BA	2614	A	C5-N7-C8	8.56	108.18	103.90
22	BA	2407	A	C5-C6-N6	8.56	130.55	123.70
22	BA	2451	A	C5-C6-N1	8.56	121.98	117.70
22	BA	2814	A	N7-C8-N9	-8.56	109.52	113.80
22	BA	1810	A	C5-C6-N6	8.55	130.54	123.70
22	BA	127	A	N3-C4-C5	-8.54	120.82	126.80
22	BA	191	A	C5-N7-C8	8.54	108.17	103.90
22	BA	730	A	C4-C5-C6	8.54	121.27	117.00
1	AA	665	A	N3-C4-C5	-8.53	120.83	126.80
22	BA	1434	A	N3-C4-C5	-8.53	120.83	126.80
22	BA	2614	A	N7-C8-N9	-8.53	109.54	113.80
22	BA	959	A	C5-N7-C8	8.52	108.16	103.90
1	AA	563	A	C4-C5-C6	8.52	121.26	117.00
22	BA	1566	A	N3-C4-C5	-8.52	120.84	126.80
22	BA	322	A	N3-C4-C5	-8.51	120.84	126.80
22	BA	781	A	C5-N7-C8	8.51	108.16	103.90
22	BA	1515	A	N7-C8-N9	-8.51	109.54	113.80
22	BA	626	A	N7-C8-N9	-8.51	109.55	113.80
22	BA	1010	A	N3-C4-C5	-8.51	120.84	126.80
55	B8	6	A	C8-N9-C4	8.51	109.20	105.80
22	BA	422	A	N7-C8-N9	-8.51	109.55	113.80
22	BA	793	A	C5-C6-N6	8.51	130.50	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	13	A	N9-C4-C5	8.50	109.20	105.80
22	BA	217	A	N7-C8-N9	-8.50	109.55	113.80
1	AA	1339	A	N3-C4-C5	-8.50	120.85	126.80
22	BA	563	A	C5-N7-C8	8.50	108.15	103.90
1	AA	1196	A	N3-C4-C5	-8.49	120.85	126.80
22	BA	943	A	N7-C8-N9	-8.49	109.55	113.80
22	BA	1359	A	N3-C4-C5	-8.49	120.86	126.80
1	AA	901	A	N7-C8-N9	-8.49	109.55	113.80
22	BA	1936	A	N7-C8-N9	-8.49	109.56	113.80
1	AA	1332	A	N3-C4-C5	-8.49	120.86	126.80
1	AA	1446	A	N7-C8-N9	-8.49	109.56	113.80
1	AA	1357	A	N7-C8-N9	-8.48	109.56	113.80
22	BA	1739	A	N7-C8-N9	-8.48	109.56	113.80
22	BA	2602	A	N3-C4-C5	-8.48	120.86	126.80
1	AA	74	A	N3-C4-C5	-8.48	120.86	126.80
22	BA	2748	A	N3-C4-C5	-8.48	120.86	126.80
1	AA	1502	A	N3-C4-C5	-8.48	120.86	126.80
22	BA	1272	A	N3-C4-C5	-8.47	120.87	126.80
22	BA	1937	A	C5-N7-C8	8.47	108.14	103.90
22	BA	2335	A	C4-C5-C6	8.46	121.23	117.00
22	BA	2274	A	N9-C4-C5	8.45	109.18	105.80
22	BA	422	A	N9-C4-C5	8.45	109.18	105.80
22	BA	829	A	N3-C4-C5	-8.45	120.88	126.80
22	BA	2225	A	N3-C4-C5	-8.45	120.89	126.80
22	BA	2725	A	N3-C4-C5	-8.44	120.89	126.80
22	BA	131	A	C5-C6-N6	8.44	130.45	123.70
22	BA	2281	A	N9-C4-C5	8.44	109.18	105.80
22	BA	262	A	C5-N7-C8	8.44	108.12	103.90
1	AA	792	A	N3-C4-C5	-8.44	120.89	126.80
1	AA	32	A	C5-C6-N6	8.43	130.44	123.70
22	BA	699	A	C5-N7-C8	8.43	108.11	103.90
22	BA	825	A	C5-N7-C8	8.43	108.11	103.90
1	AA	572	A	N3-C4-C5	-8.42	120.90	126.80
22	BA	2335	A	C5-N7-C8	8.42	108.11	103.90
22	BA	1069	A	N3-C4-C5	-8.42	120.91	126.80
22	BA	13	A	C5-N7-C8	8.42	108.11	103.90
55	B8	58	A	C5-N7-C8	8.42	108.11	103.90
22	BA	820	A	C5-N7-C8	8.40	108.10	103.90
22	BA	2741	A	N7-C8-N9	-8.40	109.60	113.80
22	BA	586	A	C5-N7-C8	8.40	108.10	103.90
22	BA	644	A	C5-N7-C8	8.40	108.10	103.90
1	AA	8	A	N3-C4-C5	-8.39	120.93	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2826	A	C5-N7-C8	8.38	108.09	103.90
1	AA	383	A	C5-C6-N6	8.38	130.41	123.70
1	AA	889	A	N9-C4-C5	8.38	109.15	105.80
22	BA	1780	A	N3-C4-C5	-8.38	120.94	126.80
22	BA	423	A	N9-C4-C5	8.37	109.15	105.80
22	BA	457	A	N9-C4-C5	8.36	109.14	105.80
22	BA	1029	A	C4-C5-C6	8.36	121.18	117.00
22	BA	2590	A	C5-N7-C8	8.36	108.08	103.90
1	AA	300	A	C5-C6-N6	8.36	130.38	123.70
22	BA	478	A	N7-C8-N9	-8.36	109.62	113.80
22	BA	1525	A	N3-C4-C5	-8.36	120.95	126.80
22	BA	783	A	N9-C4-C5	8.35	109.14	105.80
22	BA	2753	A	N9-C4-C5	8.35	109.14	105.80
22	BA	802	A	C5-N7-C8	8.35	108.08	103.90
22	BA	1285	A	C5-N7-C8	8.35	108.08	103.90
1	AA	996	A	C5-N7-C8	8.34	108.07	103.90
22	BA	975	A	N9-C4-C5	8.34	109.14	105.80
22	BA	675	A	C5-N7-C8	8.34	108.07	103.90
1	AA	520	A	C5-N7-C8	8.34	108.07	103.90
1	AA	1447	A	N3-C4-C5	-8.33	120.97	126.80
22	BA	466	A	N9-C4-C5	8.33	109.13	105.80
22	BA	1029	A	C5-N7-C8	8.33	108.07	103.90
22	BA	2051	A	N7-C8-N9	-8.33	109.63	113.80
22	BA	1265	A	N9-C4-C5	8.32	109.13	105.80
22	BA	2598	A	N9-C4-C5	8.32	109.13	105.80
22	BA	820	A	C4-C5-C6	8.32	121.16	117.00
22	BA	1469	A	C4-C5-C6	8.32	121.16	117.00
1	AA	1434	A	C5-N7-C8	8.31	108.06	103.90
22	BA	71	A	C5-N7-C8	8.31	108.06	103.90
22	BA	1393	A	N3-C4-C5	-8.31	120.98	126.80
22	BA	761	A	N9-C4-C5	8.30	109.12	105.80
1	AA	1101	A	N3-C4-C5	-8.30	120.99	126.80
22	BA	941	A	C5-N7-C8	8.29	108.05	103.90
55	B8	51	A	C5-N7-C8	8.29	108.05	103.90
22	BA	905	A	N9-C4-C5	8.29	109.12	105.80
1	AA	583	A	N9-C4-C5	8.29	109.11	105.80
22	BA	2577	A	C5-N7-C8	8.29	108.05	103.90
22	BA	2810	A	N9-C4-C5	8.29	109.12	105.80
55	B8	59	A	C5-N7-C8	8.29	108.04	103.90
22	BA	2518	A	C5-N7-C8	8.29	108.04	103.90
22	BA	1981	A	N3-C4-C5	-8.28	121.00	126.80
1	AA	574	A	N3-C4-C5	-8.28	121.01	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	38	A	C5-N7-C8	8.28	108.04	103.90
1	AA	432	A	C5-N7-C8	8.27	108.03	103.90
22	BA	311	A	N3-C4-C5	-8.27	121.02	126.80
22	BA	1269	A	C4-C5-C6	8.27	121.13	117.00
22	BA	532	A	C5-N7-C8	8.26	108.03	103.90
22	BA	1677	A	C4-C5-C6	8.26	121.13	117.00
22	BA	2799	A	N3-C4-N9	8.26	134.01	127.40
1	AA	431	A	N3-C4-C5	-8.26	121.02	126.80
22	BA	1000	A	C5-N7-C8	8.26	108.03	103.90
22	BA	1641	A	N7-C8-N9	-8.26	109.67	113.80
1	AA	1434	A	N9-C4-C5	8.26	109.10	105.80
1	AA	1513	A	N9-C4-C5	8.26	109.10	105.80
22	BA	191	A	N9-C4-C5	8.26	109.10	105.80
22	BA	1854	A	C4-C5-C6	8.26	121.13	117.00
1	AA	397	A	C5-C6-N6	8.25	130.30	123.70
55	B8	73	A	C5-N7-C8	8.25	108.03	103.90
22	BA	1205	A	N9-C4-C5	8.25	109.10	105.80
22	BA	1614	A	N9-C4-C5	8.25	109.10	105.80
22	BA	1805	A	C5-N7-C8	8.24	108.02	103.90
1	AA	706	A	C4-C5-C6	8.24	121.12	117.00
55	B8	21	A	C5-N7-C8	8.24	108.02	103.90
22	BA	507	A	N7-C8-N9	-8.24	109.68	113.80
22	BA	1597	A	C5-N7-C8	8.24	108.02	103.90
1	AA	16	A	N9-C4-C5	8.23	109.09	105.80
22	BA	655	A	N3-C4-C5	-8.22	121.04	126.80
22	BA	752	A	C5-N7-C8	8.22	108.01	103.90
1	AA	465	A	C5-C6-N1	8.22	121.81	117.70
1	AA	533	A	C4-C5-C6	8.22	121.11	117.00
22	BA	2071	A	N7-C8-N9	-8.22	109.69	113.80
22	BA	223	A	N3-C4-C5	-8.22	121.05	126.80
1	AA	412	A	N3-C4-C5	-8.22	121.05	126.80
22	BA	1890	A	C5-N7-C8	8.22	108.01	103.90
22	BA	1241	A	C5-C6-N6	8.22	130.27	123.70
22	BA	2346	A	N9-C4-C5	8.21	109.08	105.80
22	BA	1088	A	C5-N7-C8	8.21	108.01	103.90
22	BA	1419	A	N3-C4-C5	-8.21	121.05	126.80
22	BA	2837	A	C5-N7-C8	8.21	108.00	103.90
22	BA	2430	A	N9-C4-C5	8.21	109.08	105.80
22	BA	1784	A	C5-N7-C8	8.20	108.00	103.90
22	BA	2459	A	C5-N7-C8	8.20	108.00	103.90
22	BA	2766	A	C4-C5-C6	8.20	121.10	117.00
1	AA	673	A	N9-C4-C5	8.20	109.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1385	A	N3-C4-C5	-8.19	121.07	126.80
1	AA	600	A	N3-C4-C5	-8.19	121.07	126.80
1	AA	958	A	N9-C4-C5	8.19	109.07	105.80
22	BA	231	A	N9-C4-C5	8.18	109.07	105.80
22	BA	216	A	C5-N7-C8	8.18	107.99	103.90
22	BA	1253	A	N9-C4-C5	8.18	109.07	105.80
22	BA	2757	A	C4-C5-C6	8.18	121.09	117.00
22	BA	2776	A	C5-N7-C8	8.18	107.99	103.90
22	BA	2662	A	C4-C5-C6	8.18	121.09	117.00
1	AA	274	A	C8-N9-C4	8.17	109.07	105.80
22	BA	979	A	N9-C4-C5	8.17	109.07	105.80
1	AA	1046	A	C4-C5-C6	8.17	121.08	117.00
1	AA	397	A	C4-C5-C6	8.16	121.08	117.00
22	BA	216	A	N9-C4-C5	8.16	109.06	105.80
22	BA	1785	A	N3-C4-C5	-8.16	121.09	126.80
55	B8	42	A	C5-N7-C8	8.16	107.98	103.90
22	BA	1630	A	C5-N7-C8	8.16	107.98	103.90
22	BA	1847	A	N7-C8-N9	-8.16	109.72	113.80
22	BA	1427	A	N3-C4-C5	-8.16	121.09	126.80
22	BA	1614	A	N7-C8-N9	-8.16	109.72	113.80
55	B8	41	A	C5-N7-C8	8.15	107.98	103.90
22	BA	480	A	N7-C8-N9	-8.15	109.72	113.80
22	BA	1641	A	C4-C5-C6	8.15	121.08	117.00
1	AA	16	A	C5-N7-C8	8.14	107.97	103.90
22	BA	529	A	N9-C4-C5	8.14	109.06	105.80
22	BA	1672	A	C5-N7-C8	8.14	107.97	103.90
23	BB	59	A	C5-N7-C8	8.14	107.97	103.90
1	AA	371	A	C5-N7-C8	8.14	107.97	103.90
22	BA	449	A	C5-N7-C8	8.14	107.97	103.90
1	AA	499	A	C5-N7-C8	8.14	107.97	103.90
22	BA	482	A	N7-C8-N9	-8.13	109.73	113.80
22	BA	668	A	N3-C4-C5	-8.13	121.11	126.80
22	BA	2009	A	C5-N7-C8	8.13	107.97	103.90
22	BA	2101	A	N9-C4-C5	8.14	109.06	105.80
22	BA	1073	A	C5-N7-C8	8.13	107.97	103.90
22	BA	2572	A	N3-C4-C5	-8.13	121.11	126.80
22	BA	1470	A	C4-C5-C6	8.13	121.06	117.00
22	BA	927	A	C5-N7-C8	8.13	107.96	103.90
1	AA	1428	A	C5-N7-C8	8.12	107.96	103.90
1	AA	553	A	C5-N7-C8	8.12	107.96	103.90
22	BA	1598	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1375	A	C4-C5-C6	8.12	121.06	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1608	A	N7-C8-N9	-8.12	109.74	113.80
22	BA	990	A	C5-N7-C8	8.11	107.95	103.90
22	BA	1678	A	C4-C5-C6	8.11	121.06	117.00
22	BA	1789	A	N3-C4-C5	-8.11	121.12	126.80
22	BA	2761	A	N9-C4-C5	8.11	109.04	105.80
1	AA	1204	A	C5-N7-C8	8.10	107.95	103.90
22	BA	863	A	C5-C6-N6	8.10	130.18	123.70
22	BA	2433	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1500	A	N7-C8-N9	-8.10	109.75	113.80
22	BA	2450	A	N7-C8-N9	-8.09	109.75	113.80
1	AA	321	A	C5-N7-C8	8.09	107.95	103.90
22	BA	2281	A	C5-N7-C8	8.09	107.94	103.90
9	AI	11	ARG	NE-CZ-NH2	-8.09	116.26	120.30
22	BA	111	A	C5-N7-C8	8.09	107.94	103.90
22	BA	673	C	C2-N3-C4	-8.09	115.86	119.90
22	BA	203	A	N9-C4-C5	8.08	109.03	105.80
22	BA	849	A	C4-C5-C6	8.08	121.04	117.00
22	BA	1722	A	C4-C5-C6	8.08	121.04	117.00
22	BA	1286	A	C5-N7-C8	8.08	107.94	103.90
1	AA	454	G	N3-C4-N9	8.07	130.84	126.00
22	BA	1572	A	C4-C5-C6	8.07	121.04	117.00
55	B8	6	A	C5-N7-C8	8.07	107.94	103.90
22	BA	422	A	C4-C5-C6	8.07	121.03	117.00
22	BA	911	A	C4-C5-C6	8.07	121.03	117.00
22	BA	479	A	N3-C4-C5	-8.06	121.16	126.80
22	BA	2665	A	C5-N7-C8	8.06	107.93	103.90
22	BA	2005	A	C5-N7-C8	8.06	107.93	103.90
22	BA	44	A	N9-C4-C5	8.05	109.02	105.80
22	BA	1551	A	C5-N7-C8	8.05	107.93	103.90
22	BA	2726	A	N9-C4-C5	8.05	109.02	105.80
22	BA	1287	A	C5-N7-C8	8.04	107.92	103.90
1	AA	320	A	C5-N7-C8	8.04	107.92	103.90
22	BA	911	A	C5-C6-N6	8.04	130.13	123.70
1	AA	1227	A	N9-C4-C5	8.04	109.02	105.80
22	BA	1819	A	N9-C4-C5	8.04	109.01	105.80
1	AA	1188	A	N9-C4-C5	8.03	109.01	105.80
22	BA	845	A	C5-C6-N6	8.03	130.13	123.70
22	BA	2077	A	C4-C5-C6	8.04	121.02	117.00
1	AA	718	A	C4-C5-C6	8.03	121.02	117.00
22	BA	1936	A	C4-C5-C6	8.03	121.02	117.00
1	AA	1418	A	C4-C5-C6	8.03	121.01	117.00
22	BA	1528	A	C5-N7-C8	8.03	107.91	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	480	A	C4-C5-C6	8.03	121.01	117.00
22	BA	2352	A	C5-N7-C8	8.02	107.91	103.90
22	BA	512	G	O4'-C1'-N9	8.02	114.62	108.20
22	BA	751	A	C5-N7-C8	8.02	107.91	103.90
22	BA	825	A	N9-C4-C5	8.02	109.01	105.80
22	BA	1001	A	N9-C4-C5	8.02	109.01	105.80
22	BA	734	A	C5-N7-C8	8.02	107.91	103.90
22	BA	1755	A	C5-N7-C8	8.02	107.91	103.90
1	AA	781	A	C5-N7-C8	8.02	107.91	103.90
1	AA	1491	G	OP1-P-O3'	-8.01	87.58	105.20
1	AA	32	A	C4-C5-C6	8.01	121.00	117.00
1	AA	621	A	N9-C4-C5	8.01	109.00	105.80
22	BA	404	A	N3-C4-C5	-8.00	121.20	126.80
1	AA	753	A	N9-C4-C5	7.99	109.00	105.80
22	BA	352	A	N3-C4-C5	-7.99	121.21	126.80
22	BA	2447	G	C6-N1-C2	-7.99	120.31	125.10
22	BA	218	A	C4-C5-C6	7.98	120.99	117.00
1	AA	1468	A	C4-C5-C6	7.98	120.99	117.00
22	BA	84	A	N3-C4-C5	-7.98	121.22	126.80
1	AA	673	A	C4-C5-C6	7.97	120.99	117.00
22	BA	515	A	C5-N7-C8	7.97	107.89	103.90
22	BA	1545	A	N9-C4-C5	7.97	108.99	105.80
1	AA	190	A	C5-C6-N6	7.97	130.07	123.70
22	BA	2851	A	C5-N7-C8	7.97	107.88	103.90
22	BA	1431	A	C5-N7-C8	7.97	107.88	103.90
1	AA	371	A	N9-C4-C5	7.96	108.99	105.80
22	BA	526	A	N9-C4-C5	7.96	108.99	105.80
22	BA	1787	A	C5-N7-C8	7.96	107.88	103.90
22	BA	1275	A	N3-C4-C5	-7.96	121.23	126.80
22	BA	204	A	C5-N7-C8	7.96	107.88	103.90
23	BB	101	A	C5-N7-C8	7.96	107.88	103.90
22	BA	804	A	C5-N7-C8	7.96	107.88	103.90
22	BA	449	A	C4-C5-C6	7.95	120.98	117.00
22	BA	783	A	N7-C8-N9	-7.95	109.82	113.80
22	BA	2821	A	C5-N7-C8	7.95	107.88	103.90
22	BA	126	A	N3-C4-C5	-7.95	121.24	126.80
22	BA	21	A	C5-N7-C8	7.95	107.87	103.90
22	BA	1889	A	N9-C4-C5	7.95	108.98	105.80
1	AA	502	A	C4-C5-C6	7.95	120.97	117.00
1	AA	1246	A	C5-N7-C8	7.95	107.87	103.90
22	BA	764	A	N7-C8-N9	-7.95	109.83	113.80
22	BA	322	A	C5-N7-C8	7.94	107.87	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1227	A	N7-C8-N9	-7.94	109.83	113.80
22	BA	2542	A	N9-C4-C5	7.94	108.98	105.80
1	AA	74	A	C5-N7-C8	7.94	107.87	103.90
1	AA	900	A	C5-N7-C8	7.94	107.87	103.90
22	BA	207	A	N9-C4-C5	7.94	108.98	105.80
22	BA	804	A	N9-C4-C5	7.94	108.98	105.80
22	BA	2101	A	C5-N7-C8	7.94	107.87	103.90
22	BA	342	A	N9-C4-C5	7.94	108.98	105.80
1	AA	1171	A	C4-C5-C6	7.94	120.97	117.00
1	AA	1239	A	N3-C4-C5	-7.93	121.25	126.80
22	BA	2273	A	C5-N7-C8	7.93	107.87	103.90
22	BA	2513	A	N9-C4-C5	7.93	108.97	105.80
22	BA	1253	A	N7-C8-N9	-7.93	109.83	113.80
1	AA	978	A	C5-N7-C8	7.93	107.87	103.90
22	BA	2154	A	C5-N7-C8	7.93	107.86	103.90
1	AA	572	A	N9-C4-C5	7.93	108.97	105.80
1	AA	958	A	C5-N7-C8	7.93	107.86	103.90
1	AA	923	A	C4-C5-C6	7.92	120.96	117.00
22	BA	165	A	N9-C4-C5	7.92	108.97	105.80
22	BA	492	A	C4-C5-C6	7.92	120.96	117.00
8	AH	96	MET	N-CA-CB	-7.92	96.34	110.60
22	BA	479	A	N9-C4-C5	7.92	108.97	105.80
22	BA	2541	A	C5-N7-C8	7.92	107.86	103.90
22	BA	2060	A	N9-C4-C5	7.92	108.97	105.80
1	AA	583	A	C5-N7-C8	7.92	107.86	103.90
22	BA	1998	A	C5-N7-C8	7.92	107.86	103.90
1	AA	44	A	C5-N7-C8	7.91	107.86	103.90
1	AA	918	A	N9-C4-C5	7.91	108.97	105.80
22	BA	1759	A	C5-N7-C8	7.91	107.86	103.90
22	BA	1262	A	N9-C4-C5	7.91	108.97	105.80
1	AA	195	A	N9-C4-C5	7.91	108.96	105.80
22	BA	821	A	N9-C4-C5	7.91	108.96	105.80
22	BA	1194	A	C5-N7-C8	7.91	107.86	103.90
22	BA	10	A	N9-C4-C5	7.91	108.96	105.80
22	BA	483	A	C5-N7-C8	7.91	107.85	103.90
1	AA	1332	A	C8-N9-C4	7.90	108.96	105.80
22	BA	941	A	N9-C4-C5	7.90	108.96	105.80
22	BA	2700	A	C5-N7-C8	7.90	107.85	103.90
22	BA	972	A	N9-C4-C5	7.90	108.96	105.80
22	BA	1637	A	C5-N7-C8	7.90	107.85	103.90
22	BA	1189	A	C5-N7-C8	7.90	107.85	103.90
1	AA	151	A	N9-C4-C5	7.90	108.96	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	83	A	C5-N7-C8	7.90	107.85	103.90
55	B8	20	U	OP1-P-OP2	7.90	131.45	119.60
22	BA	677	A	N3-C4-N9	7.89	133.71	127.40
22	BA	1890	A	N9-C4-C5	7.89	108.96	105.80
22	BA	199	A	N9-C4-C5	7.89	108.96	105.80
22	BA	515	A	N9-C4-C5	7.89	108.96	105.80
22	BA	2820	A	N3-C4-C5	-7.89	121.28	126.80
22	BA	794	A	C5-N7-C8	7.89	107.84	103.90
22	BA	2600	A	C5-C6-N6	7.89	130.01	123.70
1	AA	949	A	C5-N7-C8	7.88	107.84	103.90
22	BA	1373	A	C4-C5-C6	7.88	120.94	117.00
22	BA	2268	A	C5-N7-C8	7.88	107.84	103.90
22	BA	457	A	C5-N7-C8	7.88	107.84	103.90
22	BA	2449	U	N3-C2-O2	-7.88	116.69	122.20
22	BA	705	A	C5-N7-C8	7.88	107.84	103.90
22	BA	160	A	N9-C4-C5	7.87	108.95	105.80
22	BA	167	A	C5-N7-C8	7.87	107.83	103.90
22	BA	1308	A	N9-C4-C5	7.87	108.95	105.80
1	AA	996	A	N9-C4-C5	7.87	108.95	105.80
22	BA	203	A	C5-N7-C8	7.87	107.83	103.90
22	BA	753	A	C5-N7-C8	7.86	107.83	103.90
22	BA	2051	A	N9-C4-C5	7.86	108.94	105.80
22	BA	1772	A	C5-N7-C8	7.86	107.83	103.90
22	BA	2835	A	C5-N7-C8	7.86	107.83	103.90
22	BA	454	A	N9-C4-C5	7.86	108.94	105.80
1	AA	596	A	C5-N7-C8	7.86	107.83	103.90
22	BA	819	A	C4-C5-C6	7.85	120.93	117.00
22	BA	347	A	C5-N7-C8	7.85	107.83	103.90
22	BA	800	A	C5-N7-C8	7.85	107.82	103.90
22	BA	2564	A	C5-N7-C8	7.85	107.83	103.90
1	AA	1238	A	N9-C4-C5	7.85	108.94	105.80
22	BA	454	A	C5-N7-C8	7.85	107.82	103.90
22	BA	917	A	C5-N7-C8	7.85	107.82	103.90
22	BA	1286	A	N9-C4-C5	7.85	108.94	105.80
1	AA	1275	A	C5-N7-C8	7.84	107.82	103.90
22	BA	819	A	C5-N7-C8	7.84	107.82	103.90
22	BA	1453	A	C5-N7-C8	7.84	107.82	103.90
1	AA	300	A	N7-C8-N9	-7.84	109.88	113.80
22	BA	502	A	N9-C4-C5	7.84	108.94	105.80
1	AA	655	A	C5-N7-C8	7.84	107.82	103.90
1	AA	397	A	N3-C4-N9	7.84	133.67	127.40
22	BA	492	A	C5-N7-C8	7.84	107.82	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	B8	20	U	N3-C4-C5	7.83	119.30	114.60
1	AA	131	A	N9-C4-C5	7.83	108.93	105.80
22	BA	2577	A	C4-C5-C6	7.83	120.92	117.00
22	BA	1553	A	C4-C5-C6	7.83	120.91	117.00
1	AA	374	A	C5-N7-C8	7.82	107.81	103.90
1	AA	792	A	C5-N7-C8	7.82	107.81	103.90
22	BA	1597	A	N9-C4-C5	7.82	108.93	105.80
22	BA	207	A	C5-N7-C8	7.82	107.81	103.90
22	BA	1275	A	C5-N7-C8	7.82	107.81	103.90
22	BA	505	A	C4-C5-C6	7.82	120.91	117.00
22	BA	905	A	C5-N7-C8	7.82	107.81	103.90
22	BA	2711	A	C5-N7-C8	7.82	107.81	103.90
1	AA	935	A	C5-N7-C8	7.81	107.81	103.90
22	BA	1431	A	C4-C5-C6	7.81	120.91	117.00
22	BA	1551	A	N9-C4-C5	7.81	108.92	105.80
1	AA	901	A	C5-N7-C8	7.81	107.81	103.90
22	BA	449	A	N9-C4-C5	7.81	108.92	105.80
22	BA	563	A	N9-C4-C5	7.81	108.92	105.80
22	BA	1586	A	C5-N7-C8	7.81	107.80	103.90
22	BA	2837	A	N9-C4-C5	7.81	108.92	105.80
22	BA	2872	A	N3-C4-C5	-7.81	121.33	126.80
1	AA	1333	A	C5-N7-C8	7.81	107.80	103.90
1	AA	533	A	C5-N7-C8	7.80	107.80	103.90
1	AA	356	A	C5-N7-C8	7.80	107.80	103.90
22	BA	2482	A	C5-N7-C8	7.80	107.80	103.90
22	BA	241	A	N9-C4-C5	7.80	108.92	105.80
22	BA	2298	A	C5-N7-C8	7.79	107.80	103.90
22	BA	2497	A	C5-N7-C8	7.79	107.80	103.90
1	AA	919	A	N9-C4-C5	7.79	108.92	105.80
22	BA	2471	A	C5-N7-C8	7.79	107.80	103.90
1	AA	915	A	C5-N7-C8	7.79	107.79	103.90
1	AA	1238	A	C5-N7-C8	7.79	107.79	103.90
1	AA	665	A	N9-C4-C5	7.79	108.91	105.80
22	BA	270	A	N9-C4-C5	7.79	108.91	105.80
22	BA	1470	A	N9-C4-C5	7.79	108.92	105.80
22	BA	1927	A	C5-N7-C8	7.79	107.79	103.90
22	BA	2095	A	C5-N7-C8	7.78	107.79	103.90
22	BA	423	A	C5-N7-C8	7.78	107.79	103.90
22	BA	528	A	C5-N7-C8	7.78	107.79	103.90
22	BA	2284	A	C4-C5-C6	7.78	120.89	117.00
22	BA	1048	A	C5-N7-C8	7.78	107.79	103.90
22	BA	2077	A	N7-C8-N9	-7.78	109.91	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	363	A	N9-C4-C5	7.78	108.91	105.80
1	AA	1480	A	N9-C4-C5	7.78	108.91	105.80
22	BA	1367	A	N9-C4-C5	7.78	108.91	105.80
1	AA	468	A	C5-N7-C8	7.77	107.79	103.90
1	AA	1375	A	C5-N7-C8	7.77	107.79	103.90
22	BA	2530	A	C4-C5-C6	7.77	120.89	117.00
1	AA	706	A	C5-N7-C8	7.77	107.78	103.90
22	BA	479	A	C5-N7-C8	7.77	107.78	103.90
22	BA	1111	A	C5-N7-C8	7.77	107.78	103.90
22	BA	973	A	N7-C8-N9	-7.76	109.92	113.80
22	BA	1786	A	C5-N7-C8	7.76	107.78	103.90
22	BA	1787	A	N3-C4-N9	7.76	133.61	127.40
22	BA	1810	A	N7-C8-N9	-7.76	109.92	113.80
55	B8	20	U	N3-C2-O2	-7.76	116.77	122.20
1	AA	622	A	N9-C4-C5	7.76	108.90	105.80
22	BA	1077	A	N9-C4-C5	7.76	108.90	105.80
22	BA	947	A	C5-N7-C8	7.76	107.78	103.90
22	BA	2632	A	C5-N7-C8	7.76	107.78	103.90
22	BA	1603	A	C5-N7-C8	7.76	107.78	103.90
22	BA	783	A	C5-N7-C8	7.75	107.78	103.90
22	BA	807	U	C2-N3-C4	-7.75	122.35	127.00
22	BA	2019	A	C5-N7-C8	7.75	107.77	103.90
1	AA	1398	A	N9-C4-C5	7.75	108.90	105.80
1	AA	1201	A	C4-C5-C6	7.74	120.87	117.00
22	BA	582	A	C5-N7-C8	7.74	107.77	103.90
1	AA	465	A	C5-N7-C8	7.74	107.77	103.90
22	BA	190	A	C5-N7-C8	7.74	107.77	103.90
22	BA	2560	A	C5-N7-C8	7.74	107.77	103.90
22	BA	608	A	C5-N7-C8	7.74	107.77	103.90
22	BA	1610	A	C5-N7-C8	7.74	107.77	103.90
1	AA	373	A	C4-C5-C6	7.73	120.87	117.00
1	AA	1213	A	C5-N7-C8	7.73	107.77	103.90
22	BA	1144	A	C5-N7-C8	7.73	107.77	103.90
22	BA	1632	A	C5-N7-C8	7.73	107.77	103.90
22	BA	572	A	C5-N7-C8	7.73	107.76	103.90
1	AA	162	A	C5-N7-C8	7.73	107.76	103.90
22	BA	2471	A	N9-C4-C5	7.73	108.89	105.80
1	AA	59	A	C5-N7-C8	7.72	107.76	103.90
22	BA	1678	A	C5-N7-C8	7.72	107.76	103.90
1	AA	872	A	N7-C8-N9	-7.72	109.94	113.80
1	AA	498	A	C5-N7-C8	7.72	107.76	103.90
22	BA	965	C	C6-N1-C2	-7.71	117.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1090	A	C5-N7-C8	7.71	107.75	103.90
22	BA	1668	A	C5-N7-C8	7.71	107.75	103.90
22	BA	2386	A	C5-N7-C8	7.71	107.75	103.90
1	AA	1418	A	C5-N7-C8	7.71	107.75	103.90
22	BA	631	A	C5-N7-C8	7.71	107.75	103.90
22	BA	1247	A	C5-N7-C8	7.70	107.75	103.90
22	BA	1679	A	C4-C5-C6	7.70	120.85	117.00
1	AA	873	A	C5-N7-C8	7.70	107.75	103.90
1	AA	408	A	C5-N7-C8	7.69	107.75	103.90
1	AA	1531	A	C4-C5-C6	7.69	120.85	117.00
22	BA	1960	A	C5-N7-C8	7.69	107.75	103.90
22	BA	255	A	C4-C5-C6	7.69	120.84	117.00
1	AA	673	A	C5-N7-C8	7.69	107.74	103.90
22	BA	196	A	C5-N7-C8	7.69	107.74	103.90
22	BA	1717	A	N9-C4-C5	7.69	108.88	105.80
22	BA	1570	A	C5-N7-C8	7.68	107.74	103.90
1	AA	246	A	C5-N7-C8	7.68	107.74	103.90
1	AA	865	A	C4-C5-C6	7.68	120.84	117.00
22	BA	2119	A	C5-N7-C8	7.68	107.74	103.90
55	B8	14	A	C5-N7-C8	7.68	107.74	103.90
22	BA	352	A	N9-C4-C5	7.68	108.87	105.80
22	BA	1469	A	C5-N7-C8	7.68	107.74	103.90
22	BA	1544	A	N9-C4-C5	7.68	108.87	105.80
22	BA	1762	A	N9-C4-C5	7.68	108.87	105.80
22	BA	2019	A	N9-C4-C5	7.68	108.87	105.80
1	AA	349	A	C5-N7-C8	7.67	107.74	103.90
22	BA	2003	A	C5-N7-C8	7.67	107.73	103.90
1	AA	1081	A	C5-N7-C8	7.67	107.73	103.90
1	AA	1495	U	N3-C2-O2	-7.67	116.83	122.20
22	BA	693	A	C5-N7-C8	7.67	107.73	103.90
1	AA	1055	A	C4-C5-C6	7.67	120.83	117.00
22	BA	2062	A	C5-N7-C8	7.67	107.73	103.90
1	AA	60	A	N9-C4-C5	7.67	108.87	105.80
1	AA	819	A	N9-C4-C5	7.67	108.87	105.80
22	BA	1029	A	N9-C4-C5	7.67	108.87	105.80
22	BA	2060	A	C5-N7-C8	7.67	107.73	103.90
22	BA	1927	A	N9-C4-C5	7.66	108.86	105.80
22	BA	960	A	C5-N7-C8	7.66	107.73	103.90
22	BA	1054	A	C5-N7-C8	7.66	107.73	103.90
1	AA	978	A	N9-C4-C5	7.66	108.86	105.80
1	AA	694	A	C5-N7-C8	7.66	107.73	103.90
22	BA	980	A	C5-N7-C8	7.66	107.73	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1679	A	C5-N7-C8	7.66	107.73	103.90
22	BA	2020	A	C5-C6-N6	7.66	129.82	123.70
55	B8	69	A	C5-N7-C8	7.66	107.73	103.90
22	BA	2134	A	C5-N7-C8	7.65	107.73	103.90
22	BA	2614	A	C4-C5-C6	7.65	120.83	117.00
22	BA	2317	A	C5-N7-C8	7.65	107.73	103.90
22	BA	104	A	C5-N7-C8	7.65	107.72	103.90
22	BA	983	A	N3-C4-C5	-7.65	121.45	126.80
22	BA	1912	A	C5-N7-C8	7.65	107.72	103.90
1	AA	1329	A	C5-N7-C8	7.64	107.72	103.90
1	AA	1410	A	C5-N7-C8	7.64	107.72	103.90
22	BA	443	A	C5-N7-C8	7.64	107.72	103.90
1	AA	197	A	C5-N7-C8	7.64	107.72	103.90
1	AA	205	A	C5-N7-C8	7.64	107.72	103.90
1	AA	1513	A	C5-N7-C8	7.64	107.72	103.90
23	BB	57	A	C4-C5-C6	7.64	120.82	117.00
1	AA	196	A	N9-C4-C5	7.64	108.85	105.80
1	AA	784	A	N9-C4-C5	7.64	108.86	105.80
22	BA	2080	A	C5-N7-C8	7.64	107.72	103.90
22	BA	2453	A	C5-N7-C8	7.64	107.72	103.90
22	BA	1032	A	N9-C4-C5	7.63	108.85	105.80
22	BA	1241	A	C5-N7-C8	7.63	107.72	103.90
22	BA	1669	A	N7-C8-N9	-7.63	109.98	113.80
22	BA	2513	A	C5-N7-C8	7.63	107.72	103.90
22	BA	2727	A	C5-N7-C8	7.63	107.72	103.90
22	BA	590	A	N9-C4-C5	7.63	108.85	105.80
22	BA	2358	A	C5-N7-C8	7.63	107.72	103.90
1	AA	1179	A	N9-C4-C5	7.63	108.85	105.80
22	BA	1194	A	N9-C4-C5	7.63	108.85	105.80
1	AA	607	A	C5-N7-C8	7.63	107.71	103.90
22	BA	574	A	N9-C4-C5	7.63	108.85	105.80
22	BA	1420	A	C5-N7-C8	7.62	107.71	103.90
22	BA	1269	A	N9-C4-C5	7.62	108.85	105.80
23	BB	75	G	C6-N1-C2	-7.62	120.53	125.10
22	BA	2448	A	N9-C4-C5	7.62	108.85	105.80
22	BA	2879	A	C5-N7-C8	7.62	107.71	103.90
22	BA	2531	A	C5-N7-C8	7.62	107.71	103.90
22	BA	2749	A	N9-C4-C5	7.62	108.85	105.80
55	B8	21	A	C4-C5-C6	7.62	120.81	117.00
1	AA	1046	A	C5-N7-C8	7.62	107.71	103.90
22	BA	1366	A	N9-C4-C5	7.62	108.85	105.80
22	BA	1668	A	N9-C4-C5	7.62	108.85	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2297	A	C5-N7-C8	7.62	107.71	103.90
1	AA	704	A	N9-C4-C5	7.61	108.84	105.80
1	AA	1022	A	C5-N7-C8	7.61	107.70	103.90
1	AA	129	A	N9-C4-C5	7.61	108.84	105.80
1	AA	1441	A	C5-N7-C8	7.61	107.70	103.90
22	BA	1829	A	C5-N7-C8	7.60	107.70	103.90
1	AA	1311	A	C5-N7-C8	7.60	107.70	103.90
22	BA	1050	A	C5-N7-C8	7.60	107.70	103.90
22	BA	1490	A	C5-N7-C8	7.60	107.70	103.90
41	BT	1	MET	N-CA-C	7.60	131.52	111.00
22	BA	52	A	C4-C5-C6	7.60	120.80	117.00
22	BA	925	A	C5-N7-C8	7.60	107.70	103.90
22	BA	627	A	C5-N7-C8	7.60	107.70	103.90
1	AA	487	A	C4-C5-C6	7.59	120.80	117.00
22	BA	1889	A	C5-N7-C8	7.59	107.70	103.90
22	BA	2753	A	C5-N7-C8	7.59	107.70	103.90
22	BA	1630	A	N9-C4-C5	7.59	108.84	105.80
1	AA	430	A	C5-N7-C8	7.59	107.69	103.90
1	AA	1180	A	N9-C4-C5	7.59	108.84	105.80
22	BA	401	A	C5-N7-C8	7.59	107.69	103.90
22	BA	751	A	C4-C5-C6	7.59	120.80	117.00
22	BA	504	A	N3-C4-C5	-7.59	121.49	126.80
22	BA	2434	A	C5-N7-C8	7.59	107.69	103.90
1	AA	1216	A	N9-C4-C5	7.58	108.83	105.80
1	AA	408	A	N9-C4-C5	7.58	108.83	105.80
22	BA	1069	A	C5-N7-C8	7.58	107.69	103.90
22	BA	2366	A	C5-N7-C8	7.58	107.69	103.90
1	AA	313	A	C5-N7-C8	7.58	107.69	103.90
22	BA	1327	A	C5-N7-C8	7.58	107.69	103.90
1	AA	1201	A	C5-C6-N1	7.58	121.49	117.70
22	BA	1470	A	C5-N7-C8	7.58	107.69	103.90
22	BA	172	A	C5-N7-C8	7.58	107.69	103.90
22	BA	655	A	C5-N7-C8	7.58	107.69	103.90
22	BA	1213	A	C5-N7-C8	7.58	107.69	103.90
22	BA	2706	A	N9-C4-C5	7.58	108.83	105.80
1	AA	77	A	C4-C5-C6	7.57	120.79	117.00
1	AA	969	A	C5-N7-C8	7.57	107.69	103.90
1	AA	1035	A	C5-N7-C8	7.57	107.69	103.90
1	AA	1465	A	C4-C5-C6	7.57	120.79	117.00
22	BA	428	A	C5-N7-C8	7.57	107.69	103.90
22	BA	1505	A	C5-N7-C8	7.57	107.69	103.90
22	BA	2766	A	C5-N7-C8	7.57	107.69	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	84	A	N9-C4-C5	7.57	108.83	105.80
22	BA	973	A	N9-C4-C5	7.57	108.83	105.80
22	BA	1353	A	C4-C5-N7	-7.57	106.92	110.70
22	BA	2602	A	C5-N7-C8	7.57	107.69	103.90
22	BA	2734	A	C5-N7-C8	7.57	107.69	103.90
22	BA	644	A	C4-C5-C6	7.57	120.78	117.00
22	BA	1246	A	C5-N7-C8	7.57	107.68	103.90
1	AA	873	A	C4-C5-C6	7.57	120.78	117.00
22	BA	181	A	C5-N7-C8	7.57	107.68	103.90
22	BA	1165	A	N9-C4-C5	7.57	108.83	105.80
22	BA	2051	A	C4-C5-C6	7.57	120.78	117.00
23	BB	99	A	C5-N7-C8	7.57	107.68	103.90
22	BA	2614	A	C4-C5-N7	-7.56	106.92	110.70
1	AA	572	A	C5-N7-C8	7.56	107.68	103.90
1	AA	1374	A	C5-N7-C8	7.56	107.68	103.90
22	BA	706	A	C5-N7-C8	7.56	107.68	103.90
22	BA	1504	A	C5-N7-C8	7.56	107.68	103.90
1	AA	1476	A	N9-C4-C5	7.56	108.82	105.80
22	BA	753	A	C4-C5-C6	7.56	120.78	117.00
22	BA	1403	A	C5-N7-C8	7.56	107.68	103.90
22	BA	2482	A	C4-C5-C6	7.56	120.78	117.00
1	AA	676	A	C5-N7-C8	7.56	107.68	103.90
22	BA	1749	A	C5-N7-C8	7.56	107.68	103.90
22	BA	1749	A	N9-C4-C5	7.56	108.82	105.80
22	BA	2270	A	N9-C4-C5	7.56	108.82	105.80
1	AA	743	A	C4-C5-C6	7.56	120.78	117.00
1	AA	28	A	C4-C5-C6	7.55	120.78	117.00
22	BA	149	A	N9-C4-C5	7.55	108.82	105.80
22	BA	1794	A	C5-N7-C8	7.55	107.68	103.90
22	BA	2721	A	C5-N7-C8	7.55	107.67	103.90
22	BA	2108	A	C4-C5-C6	7.55	120.78	117.00
22	BA	676	A	N9-C4-C5	7.55	108.82	105.80
22	BA	2727	A	C4-C5-C6	7.55	120.77	117.00
1	AA	579	A	N9-C4-C5	7.55	108.82	105.80
22	BA	1302	A	C5-N7-C8	7.55	107.67	103.90
22	BA	1147	A	C5-N7-C8	7.54	107.67	103.90
23	BB	57	A	C5-N7-C8	7.54	107.67	103.90
22	BA	2247	A	C5-N7-C8	7.54	107.67	103.90
22	BA	2266	A	N9-C4-C5	7.54	108.82	105.80
1	AA	320	A	N9-C4-C5	7.54	108.81	105.80
22	BA	1247	A	N9-C4-C5	7.54	108.81	105.80
1	AA	19	A	N9-C4-C5	7.53	108.81	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	920	A	C5-N7-C8	7.53	107.67	103.90
23	BB	58	A	C5-N7-C8	7.53	107.67	103.90
1	AA	152	A	N9-C4-C5	7.53	108.81	105.80
1	AA	1332	A	C5-N7-C8	7.53	107.67	103.90
22	BA	146	A	C5-N7-C8	7.53	107.67	103.90
1	AA	353	A	C5-N7-C8	7.53	107.66	103.90
1	AA	1428	A	N9-C4-C5	7.53	108.81	105.80
22	BA	2740	A	C5-N7-C8	7.53	107.67	103.90
1	AA	642	A	C5-N7-C8	7.53	107.66	103.90
22	BA	152	A	C4-C5-C6	7.53	120.76	117.00
22	BA	792	A	C4-C5-C6	7.53	120.76	117.00
22	BA	2094	A	C5-N7-C8	7.53	107.66	103.90
1	AA	452	A	C5-N7-C8	7.53	107.66	103.90
22	BA	1853	A	C5-N7-C8	7.53	107.66	103.90
22	BA	2173	A	C5-N7-C8	7.53	107.66	103.90
22	BA	2418	A	C5-N7-C8	7.53	107.66	103.90
55	B8	76	A	C5-N7-C8	7.53	107.66	103.90
22	BA	2778	A	C5-N7-C8	7.52	107.66	103.90
1	AA	1225	A	C5-N7-C8	7.52	107.66	103.90
22	BA	2706	A	C4-C5-C6	7.52	120.76	117.00
23	BB	53	A	C5-N7-C8	7.52	107.66	103.90
22	BA	802	A	C4-C5-C6	7.52	120.76	117.00
22	BA	1021	A	C5-N7-C8	7.52	107.66	103.90
22	BA	1322	A	C5-N7-C8	7.52	107.66	103.90
1	AA	430	A	C4-C5-C6	7.52	120.76	117.00
22	BA	735	A	C5-N7-C8	7.52	107.66	103.90
22	BA	863	A	C4-C5-C6	7.51	120.76	117.00
22	BA	1366	A	C5-N7-C8	7.51	107.66	103.90
22	BA	866	A	C5-N7-C8	7.51	107.66	103.90
22	BA	1392	A	N9-C4-C5	7.51	108.81	105.80
1	AA	325	A	C4-C5-C6	7.51	120.75	117.00
1	AA	1019	A	C5-N7-C8	7.51	107.66	103.90
22	BA	1772	A	N9-C4-C5	7.51	108.80	105.80
22	BA	2657	A	N9-C4-C5	7.51	108.80	105.80
22	BA	1088	A	C4-C5-C6	7.50	120.75	117.00
22	BA	1264	A	C5-N7-C8	7.50	107.65	103.90
22	BA	1744	A	C5-N7-C8	7.50	107.65	103.90
22	BA	2736	A	C5-N7-C8	7.50	107.65	103.90
1	AA	373	A	C5-N7-C8	7.50	107.65	103.90
1	AA	431	A	C5-N7-C8	7.50	107.65	103.90
22	BA	2835	A	N9-C4-C5	7.50	108.80	105.80
23	BB	29	A	C5-N7-C8	7.50	107.65	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	833	A	C4-C5-C6	7.50	120.75	117.00
1	AA	1197	A	C4-C5-C6	7.50	120.75	117.00
22	BA	2031	A	C5-N7-C8	7.50	107.65	103.90
22	BA	2439	A	N9-C4-C5	7.50	108.80	105.80
1	AA	1016	A	C5-N7-C8	7.49	107.65	103.90
22	BA	1384	A	N9-C4-C5	7.49	108.80	105.80
22	BA	429	A	C5-N7-C8	7.49	107.65	103.90
22	BA	1787	A	C4-C5-C6	7.49	120.75	117.00
22	BA	2033	A	C5-N7-C8	7.49	107.64	103.90
22	BA	2094	A	N9-C4-C5	7.49	108.80	105.80
1	AA	435	A	C5-N7-C8	7.49	107.64	103.90
1	AA	825	A	C5-N7-C8	7.49	107.64	103.90
1	AA	1180	A	C5-N7-C8	7.49	107.64	103.90
1	AA	1360	A	N9-C4-C5	7.49	108.80	105.80
22	BA	2241	A	C5-N7-C8	7.49	107.64	103.90
22	BA	2634	A	C5-N7-C8	7.49	107.64	103.90
22	BA	1676	A	C5-N7-C8	7.49	107.64	103.90
1	AA	949	A	N9-C4-C5	7.49	108.79	105.80
22	BA	103	A	C5-N7-C8	7.49	107.64	103.90
22	BA	1689	A	C5-N7-C8	7.48	107.64	103.90
1	AA	1429	A	C5-N7-C8	7.48	107.64	103.90
22	BA	1272	A	C5-N7-C8	7.48	107.64	103.90
22	BA	2412	A	C5-N7-C8	7.48	107.64	103.90
22	BA	470	A	C4-C5-C6	7.48	120.74	117.00
22	BA	547	A	C5-N7-C8	7.48	107.64	103.90
22	BA	2868	A	C5-N7-C8	7.48	107.64	103.90
1	AA	129	A	C5-N7-C8	7.48	107.64	103.90
1	AA	383	A	N3-C4-N9	7.48	133.38	127.40
1	AA	777	A	C5-N7-C8	7.48	107.64	103.90
22	BA	892	A	C5-N7-C8	7.48	107.64	103.90
22	BA	2163	A	C5-N7-C8	7.48	107.64	103.90
22	BA	2278	A	C5-N7-C8	7.48	107.64	103.90
1	AA	131	A	C5-N7-C8	7.47	107.64	103.90
22	BA	401	A	C4-C5-C6	7.47	120.74	117.00
22	BA	1260	A	N9-C4-C5	7.47	108.79	105.80
22	BA	1829	A	C4-C5-C6	7.47	120.74	117.00
22	BA	1987	A	C5-N7-C8	7.47	107.64	103.90
22	BA	2369	A	C5-N7-C8	7.47	107.64	103.90
22	BA	2700	A	N9-C4-C5	7.47	108.79	105.80
22	BA	2873	A	C5-N7-C8	7.47	107.64	103.90
1	AA	336	A	C5-N7-C8	7.47	107.63	103.90
1	AA	1269	A	C5-N7-C8	7.47	107.63	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1357	A	C4-C5-C6	7.47	120.73	117.00
22	BA	984	A	C5-N7-C8	7.47	107.64	103.90
22	BA	2314	A	C5-N7-C8	7.47	107.64	103.90
1	AA	414	A	C5-N7-C8	7.47	107.63	103.90
1	AA	143	A	C5-N7-C8	7.47	107.63	103.90
1	AA	451	A	C5-N7-C8	7.47	107.63	103.90
1	AA	906	A	C5-N7-C8	7.47	107.63	103.90
1	AA	938	A	C4-C5-C6	7.47	120.73	117.00
22	BA	2014	A	C5-N7-C8	7.47	107.63	103.90
1	AA	640	A	C5-N7-C8	7.46	107.63	103.90
1	AA	1036	A	C5-N7-C8	7.46	107.63	103.90
1	AA	1248	A	N9-C4-C5	7.46	108.79	105.80
22	BA	1586	A	N9-C4-C5	7.46	108.79	105.80
22	BA	1677	A	C5-N7-C8	7.46	107.63	103.90
1	AA	466	A	C5-N7-C8	7.46	107.63	103.90
1	AA	509	A	N9-C4-C5	7.46	108.78	105.80
22	BA	477	A	C4-C5-C6	7.46	120.73	117.00
22	BA	685	A	C5-N7-C8	7.46	107.63	103.90
22	BA	2733	A	C5-N7-C8	7.46	107.63	103.90
22	BA	1086	A	C5-N7-C8	7.46	107.63	103.90
22	BA	1262	A	C5-N7-C8	7.46	107.63	103.90
1	AA	223	A	C4-C5-C6	7.46	120.73	117.00
22	BA	900	A	C5-N7-C8	7.46	107.63	103.90
23	BB	101	A	N9-C4-C5	7.46	108.78	105.80
22	BA	190	A	C4-C5-C6	7.46	120.73	117.00
22	BA	1169	A	C5-N7-C8	7.46	107.63	103.90
22	BA	2198	A	C5-N7-C8	7.46	107.63	103.90
1	AA	712	A	C5-N7-C8	7.46	107.63	103.90
1	AA	1503	A	C5-N7-C8	7.46	107.63	103.90
1	AA	1219	A	C4-C5-C6	7.45	120.73	117.00
22	BA	643	A	C5-N7-C8	7.45	107.63	103.90
22	BA	820	A	N9-C4-C5	7.45	108.78	105.80
22	BA	1495	A	N9-C4-C5	7.45	108.78	105.80
22	BA	2497	A	C4-C5-C6	7.45	120.73	117.00
23	BB	46	A	C5-N7-C8	7.45	107.63	103.90
1	AA	120	A	C5-N7-C8	7.45	107.63	103.90
22	BA	217	A	C4-C5-C6	7.45	120.73	117.00
1	AA	356	A	C4-C5-C6	7.45	120.72	117.00
1	AA	1251	A	N9-C4-C5	7.45	108.78	105.80
22	BA	190	A	N9-C4-C5	7.45	108.78	105.80
1	AA	913	A	N9-C4-C5	7.45	108.78	105.80
1	AA	1016	A	N9-C4-C5	7.45	108.78	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1346	A	N9-C4-C5	7.45	108.78	105.80
22	BA	2497	A	N9-C4-C5	7.45	108.78	105.80
1	AA	149	A	N9-C4-C5	7.44	108.78	105.80
1	AA	579	A	C4-C5-C6	7.44	120.72	117.00
22	BA	1070	A	C5-N7-C8	7.44	107.62	103.90
22	BA	1244	A	C5-N7-C8	7.44	107.62	103.90
22	BA	1504	A	N9-C4-C5	7.44	108.78	105.80
1	AA	151	A	C5-N7-C8	7.44	107.62	103.90
1	AA	602	A	C5-N7-C8	7.44	107.62	103.90
22	BA	1821	A	C5-N7-C8	7.44	107.62	103.90
22	BA	2287	A	C5-N7-C8	7.44	107.62	103.90
22	BA	2670	A	C5-N7-C8	7.44	107.62	103.90
23	BB	78	A	C5-N7-C8	7.44	107.62	103.90
1	AA	2	A	C5-N7-C8	7.43	107.62	103.90
1	AA	784	A	C5-N7-C8	7.43	107.62	103.90
22	BA	5	A	C5-N7-C8	7.43	107.62	103.90
22	BA	988	A	C5-N7-C8	7.43	107.62	103.90
1	AA	415	A	C4-C5-C6	7.43	120.72	117.00
1	AA	1167	A	C5-N7-C8	7.43	107.62	103.90
1	AA	1340	A	N3-C4-C5	-7.43	121.60	126.80
22	BA	845	A	C4-C5-C6	7.43	120.72	117.00
1	AA	546	A	N9-C4-C5	7.43	108.77	105.80
1	AA	994	A	C5-N7-C8	7.43	107.61	103.90
1	AA	7	A	C5-N7-C8	7.43	107.61	103.90
1	AA	959	A	C5-N7-C8	7.43	107.61	103.90
22	BA	572	A	C4-C5-C6	7.43	120.71	117.00
22	BA	1084	A	C5-N7-C8	7.43	107.61	103.90
22	BA	1276	A	C4-C5-C6	7.43	120.71	117.00
22	BA	1664	A	N3-C4-N9	7.43	133.34	127.40
22	BA	83	A	N9-C4-C5	7.42	108.77	105.80
22	BA	2082	A	C5-N7-C8	7.42	107.61	103.90
1	AA	547	A	C5-N7-C8	7.42	107.61	103.90
1	AA	1130	A	N9-C4-C5	7.42	108.77	105.80
22	BA	1274	A	C5-N7-C8	7.42	107.61	103.90
22	BA	1583	A	C5-N7-C8	7.42	107.61	103.90
1	AA	607	A	N9-C4-C5	7.42	108.77	105.80
1	AA	1251	A	C5-N7-C8	7.42	107.61	103.90
1	AA	1340	A	C8-N9-C4	7.42	108.77	105.80
22	BA	1205	A	C5-N7-C8	7.42	107.61	103.90
1	AA	1368	A	C5-N7-C8	7.42	107.61	103.90
22	BA	1548	A	C5-N7-C8	7.42	107.61	103.90
1	AA	546	A	C5-N7-C8	7.42	107.61	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	729	A	N9-C4-C5	7.42	108.77	105.80
22	BA	1434	A	C5-N7-C8	7.42	107.61	103.90
22	BA	1981	A	C5-N7-C8	7.42	107.61	103.90
22	BA	2434	A	N9-C4-C5	7.42	108.77	105.80
22	BA	2826	A	N9-C4-C5	7.42	108.77	105.80
1	AA	363	A	C5-N7-C8	7.41	107.61	103.90
22	BA	2469	A	C5-C6-N1	7.41	121.41	117.70
1	AA	1093	A	N9-C4-C5	7.41	108.77	105.80
1	AA	1014	A	N9-C4-C5	7.41	108.76	105.80
1	AA	1110	A	N9-C4-C5	7.41	108.76	105.80
1	AA	1360	A	C5-N7-C8	7.41	107.61	103.90
22	BA	125	A	C5-N7-C8	7.41	107.61	103.90
22	BA	191	A	C4-C5-C6	7.41	120.70	117.00
22	BA	432	A	C5-N7-C8	7.41	107.61	103.90
22	BA	742	A	C5-N7-C8	7.41	107.61	103.90
1	AA	171	A	N9-C4-C5	7.41	108.76	105.80
22	BA	91	A	C5-N7-C8	7.41	107.60	103.90
22	BA	2317	A	N9-C4-C5	7.41	108.76	105.80
1	AA	1170	A	C5-N7-C8	7.41	107.60	103.90
1	AA	1492	A	N9-C4-C5	7.41	108.76	105.80
22	BA	2184	A	C5-N7-C8	7.41	107.60	103.90
1	AA	1398	A	C5-N7-C8	7.40	107.60	103.90
22	BA	1876	A	C5-N7-C8	7.40	107.60	103.90
1	AA	465	A	N3-C4-C5	-7.40	121.62	126.80
1	AA	579	A	C5-N7-C8	7.40	107.60	103.90
22	BA	2764	A	C5-N7-C8	7.40	107.60	103.90
23	BB	52	A	C5-N7-C8	7.40	107.60	103.90
1	AA	26	A	C5-N7-C8	7.40	107.60	103.90
1	AA	66	A	N9-C4-C5	7.40	108.76	105.80
1	AA	675	A	C5-N7-C8	7.40	107.60	103.90
22	BA	2792	A	C5-N7-C8	7.40	107.60	103.90
1	AA	1306	A	C4-C5-C6	7.40	120.70	117.00
22	BA	2142	A	C4-C5-C6	7.40	120.70	117.00
1	AA	938	A	C5-N7-C8	7.39	107.60	103.90
1	AA	1229	A	C5-N7-C8	7.39	107.60	103.90
1	AA	336	A	N9-C4-C5	7.39	108.76	105.80
22	BA	792	A	C5-N7-C8	7.39	107.60	103.90
1	AA	1111	A	C5-N7-C8	7.39	107.60	103.90
22	BA	89	A	C5-N7-C8	7.39	107.60	103.90
22	BA	1014	A	C5-N7-C8	7.39	107.60	103.90
22	BA	1328	A	C5-N7-C8	7.39	107.60	103.90
1	AA	19	A	C5-N7-C8	7.39	107.59	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	374	A	N9-C4-C5	7.39	108.76	105.80
22	BA	44	A	C5-N7-C8	7.39	107.59	103.90
22	BA	270	A	C5-N7-C8	7.39	107.59	103.90
22	BA	1046	A	C5-N7-C8	7.39	107.59	103.90
22	BA	782	A	N9-C4-C5	7.39	108.75	105.80
22	BA	1284	A	N9-C4-C5	7.39	108.75	105.80
22	BA	1679	A	N9-C4-C5	7.39	108.75	105.80
22	BA	947	A	C4-C5-C6	7.39	120.69	117.00
22	BA	2311	A	C5-N7-C8	7.39	107.59	103.90
22	BA	2882	A	C4-C5-N7	-7.39	107.01	110.70
23	BB	58	A	C4-C5-C6	7.38	120.69	117.00
22	BA	1189	A	C4-C5-C6	7.38	120.69	117.00
22	BA	1265	A	C5-N7-C8	7.38	107.59	103.90
22	BA	2070	A	C5-N7-C8	7.38	107.59	103.90
22	BA	2288	A	C5-N7-C8	7.38	107.59	103.90
1	AA	478	A	C5-N7-C8	7.38	107.59	103.90
22	BA	165	A	C5-N7-C8	7.38	107.59	103.90
1	AA	223	A	C5-N7-C8	7.38	107.59	103.90
1	AA	1256	A	C5-N7-C8	7.38	107.59	103.90
22	BA	255	A	C5-N7-C8	7.38	107.59	103.90
22	BA	111	A	N9-C4-C5	7.38	108.75	105.80
22	BA	1439	A	C5-N7-C8	7.38	107.59	103.90
22	BA	2411	A	N9-C4-C5	7.38	108.75	105.80
22	BA	1802	A	C5-N7-C8	7.38	107.59	103.90
22	BA	371	A	C5-N7-C8	7.37	107.59	103.90
22	BA	821	A	C5-N7-C8	7.37	107.59	103.90
22	BA	1420	A	N9-C4-C5	7.37	108.75	105.80
1	AA	906	A	N9-C4-C5	7.37	108.75	105.80
1	AA	908	A	C5-N7-C8	7.37	107.58	103.90
22	BA	222	A	C5-N7-C8	7.37	107.59	103.90
22	BA	422	A	C5-N7-C8	7.37	107.59	103.90
22	BA	2635	A	C5-N7-C8	7.37	107.58	103.90
1	AA	790	A	C4-C5-C6	7.37	120.69	117.00
22	BA	718	A	C5-N7-C8	7.37	107.58	103.90
1	AA	366	A	N9-C4-C5	7.37	108.75	105.80
1	AA	1163	A	C5-N7-C8	7.37	107.58	103.90
1	AA	1254	A	C5-N7-C8	7.37	107.58	103.90
22	BA	2309	A	C5-N7-C8	7.37	107.58	103.90
22	BA	2425	A	C5-N7-C8	7.37	107.58	103.90
1	AA	2	A	N9-C4-C5	7.37	108.75	105.80
1	AA	1465	A	C5-N7-C8	7.37	107.58	103.90
22	BA	2411	A	C5-N7-C8	7.37	107.58	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	109	A	C5-N7-C8	7.37	107.58	103.90
22	BA	899	A	C5-N7-C8	7.36	107.58	103.90
1	AA	1377	A	C5-N7-C8	7.36	107.58	103.90
1	AA	179	A	N9-C4-C5	7.36	108.75	105.80
1	AA	461	A	N3-C4-N9	7.36	133.29	127.40
1	AA	1508	A	C4-C5-C6	7.36	120.68	117.00
22	BA	861	A	C4-C5-C6	7.36	120.68	117.00
22	BA	2191	A	N9-C4-C5	7.36	108.74	105.80
22	BA	2587	A	N1-C6-N6	-7.36	114.18	118.60
23	BB	46	A	N9-C4-C5	7.36	108.74	105.80
22	BA	592	A	C5-N7-C8	7.36	107.58	103.90
1	AA	1004	A	N9-C4-C5	7.36	108.74	105.80
22	BA	2711	A	N9-C4-C5	7.36	108.74	105.80
1	AA	1374	A	C4-C5-C6	7.36	120.68	117.00
22	BA	2516	A	C5-N7-C8	7.36	107.58	103.90
1	AA	448	A	C4-C5-C6	7.35	120.68	117.00
22	BA	1067	A	C5-N7-C8	7.35	107.58	103.90
1	AA	119	A	N9-C4-C5	7.35	108.74	105.80
22	BA	1596	A	C5-N7-C8	7.35	107.58	103.90
1	AA	918	A	C5-N7-C8	7.35	107.58	103.90
1	AA	1169	A	C5-N7-C8	7.35	107.58	103.90
1	AA	1500	A	N9-C4-C5	7.35	108.74	105.80
22	BA	1552	A	C5-N7-C8	7.35	107.58	103.90
22	BA	1285	A	C4-C5-N7	-7.35	107.03	110.70
1	AA	1101	A	C5-N7-C8	7.35	107.57	103.90
22	BA	2407	A	C4-C5-C6	7.35	120.67	117.00
1	AA	787	A	C5-N7-C8	7.34	107.57	103.90
1	AA	676	A	N9-C4-C5	7.34	108.74	105.80
1	AA	845	A	C5-N7-C8	7.34	107.57	103.90
22	BA	990	A	N9-C4-C5	7.34	108.74	105.80
1	AA	781	A	N9-C4-C5	7.34	108.74	105.80
22	BA	750	A	C5-N7-C8	7.34	107.57	103.90
22	BA	1700	A	C5-N7-C8	7.34	107.57	103.90
22	BA	1791	A	N9-C4-C5	7.34	108.74	105.80
22	BA	2270	A	C5-N7-C8	7.34	107.57	103.90
1	AA	1067	A	C5-N7-C8	7.34	107.57	103.90
22	BA	52	A	C5-N7-C8	7.34	107.57	103.90
22	BA	1214	A	C5-N7-C8	7.34	107.57	103.90
22	BA	1701	A	C5-N7-C8	7.34	107.57	103.90
22	BA	1808	A	C5-N7-C8	7.34	107.57	103.90
22	BA	1810	A	N3-C4-N9	7.34	133.27	127.40
22	BA	1509	A	C5-N7-C8	7.34	107.57	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	199	A	C4-C5-C6	7.34	120.67	117.00
1	AA	1005	A	C5-N7-C8	7.34	107.57	103.90
22	BA	1089	A	C5-N7-C8	7.34	107.57	103.90
22	BA	2097	A	C4-C5-C6	7.34	120.67	117.00
22	BA	920	A	N9-C4-C5	7.33	108.73	105.80
1	AA	746	A	C4-C5-C6	7.33	120.67	117.00
22	BA	279	A	C5-N7-C8	7.33	107.57	103.90
22	BA	1085	A	C5-N7-C8	7.33	107.57	103.90
22	BA	2478	A	C5-N7-C8	7.33	107.57	103.90
22	BA	2850	A	N9-C4-C5	7.33	108.73	105.80
1	AA	306	A	C5-N7-C8	7.33	107.57	103.90
1	AA	441	A	C5-N7-C8	7.33	107.57	103.90
22	BA	1048	A	C4-C5-C6	7.33	120.67	117.00
1	AA	794	A	C5-N7-C8	7.33	107.56	103.90
22	BA	2241	A	C4-C5-C6	7.33	120.67	117.00
22	BA	2761	A	C5-N7-C8	7.33	107.56	103.90
22	BA	1342	A	C5-N7-C8	7.33	107.56	103.90
22	BA	1668	A	N3-C4-C5	-7.33	121.67	126.80
22	BA	340	A	C5-N7-C8	7.32	107.56	103.90
22	BA	2158	A	C5-N7-C8	7.32	107.56	103.90
1	AA	983	A	C4-C5-C6	7.32	120.66	117.00
22	BA	94	A	C5-N7-C8	7.32	107.56	103.90
22	BA	1241	A	N3-C4-N9	7.32	133.26	127.40
22	BA	1347	A	C5-N7-C8	7.32	107.56	103.90
22	BA	1387	A	C4-C5-C6	7.32	120.66	117.00
22	BA	2082	A	C4-C5-C6	7.32	120.66	117.00
22	BA	1773	A	C5-N7-C8	7.32	107.56	103.90
22	BA	1853	A	N9-C4-C5	7.32	108.73	105.80
22	BA	1634	A	N9-C4-C5	7.32	108.73	105.80
1	AA	382	A	C5-N7-C8	7.32	107.56	103.90
23	BB	119	A	C5-N7-C8	7.32	107.56	103.90
55	B8	58	A	C8-N9-C4	7.32	108.73	105.80
22	BA	101	A	N3-C4-N9	7.31	133.25	127.40
1	AA	814	A	C5-N7-C8	7.31	107.56	103.90
1	AA	1152	A	C5-N7-C8	7.31	107.56	103.90
1	AA	1152	A	N9-C4-C5	7.31	108.72	105.80
22	BA	217	A	C5-N7-C8	7.31	107.56	103.90
1	AA	1287	A	N9-C4-C5	7.31	108.72	105.80
22	BA	213	A	C5-N7-C8	7.31	107.56	103.90
22	BA	522	A	C4-C5-C6	7.31	120.66	117.00
22	BA	2314	A	N9-C4-C5	7.31	108.72	105.80
22	BA	2706	A	C5-N7-C8	7.31	107.55	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1413	A	N9-C4-C5	7.31	108.72	105.80
22	BA	1525	A	C5-N7-C8	7.31	107.55	103.90
22	BA	2241	A	N9-C4-C5	7.31	108.72	105.80
22	BA	2725	A	C5-N7-C8	7.31	107.55	103.90
1	AA	101	A	C5-N7-C8	7.30	107.55	103.90
22	BA	1307	A	C5-N7-C8	7.30	107.55	103.90
1	AA	243	A	C5-N7-C8	7.30	107.55	103.90
22	BA	1365	A	C5-N7-C8	7.30	107.55	103.90
1	AA	461	A	C4-C5-C6	7.30	120.65	117.00
22	BA	176	A	C5-N7-C8	7.30	107.55	103.90
22	BA	1978	A	C5-N7-C8	7.30	107.55	103.90
1	AA	559	A	C4-C5-C6	7.30	120.65	117.00
1	AA	452	A	N9-C4-C5	7.30	108.72	105.80
1	AA	1004	A	C5-N7-C8	7.30	107.55	103.90
22	BA	142	A	C5-N7-C8	7.30	107.55	103.90
22	BA	2547	A	C5-N7-C8	7.30	107.55	103.90
22	BA	2850	A	C5-N7-C8	7.30	107.55	103.90
1	AA	919	A	C5-N7-C8	7.29	107.55	103.90
22	BA	1260	A	C5-N7-C8	7.29	107.55	103.90
22	BA	761	A	N7-C8-N9	-7.29	110.15	113.80
22	BA	1080	A	C5-N7-C8	7.29	107.55	103.90
22	BA	2080	A	N9-C4-C5	7.29	108.72	105.80
22	BA	2381	A	C5-N7-C8	7.29	107.55	103.90
23	BB	109	A	N9-C4-C5	7.29	108.72	105.80
22	BA	251	A	N7-C8-N9	-7.29	110.16	113.80
22	BA	1655	A	C5-N7-C8	7.29	107.55	103.90
22	BA	2327	A	C5-N7-C8	7.29	107.55	103.90
22	BA	1084	A	C4-C5-C6	7.29	120.64	117.00
1	AA	190	A	N3-C4-N9	7.29	133.23	127.40
22	BA	2247	A	C4-C5-C6	7.29	120.64	117.00
22	BA	2758	A	N9-C4-C5	7.29	108.72	105.80
22	BA	2679	A	C5-N7-C8	7.29	107.54	103.90
1	AA	189	A	C5-N7-C8	7.29	107.54	103.90
1	AA	560	A	C5-N7-C8	7.29	107.54	103.90
22	BA	149	A	C4-C5-C6	7.29	120.64	117.00
22	BA	1579	A	N9-C4-C5	7.29	108.71	105.80
22	BA	1780	A	C5-N7-C8	7.29	107.54	103.90
22	BA	2799	A	C5-C6-N6	7.29	129.53	123.70
22	BA	344	A	N9-C4-C5	7.28	108.71	105.80
22	BA	1039	A	N9-C4-C5	7.28	108.71	105.80
22	BA	1080	A	N9-C4-C5	7.28	108.71	105.80
1	AA	1287	A	C5-N7-C8	7.28	107.54	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	504	A	C5-N7-C8	7.28	107.54	103.90
22	BA	2733	A	N9-C4-C5	7.28	108.71	105.80
1	AA	1368	A	N9-C4-C5	7.28	108.71	105.80
22	BA	503	A	N9-C4-C5	7.28	108.71	105.80
22	BA	2212	A	C5-N7-C8	7.28	107.54	103.90
22	BA	2860	A	N9-C4-C5	7.28	108.71	105.80
1	AA	1163	A	C4-C5-C6	7.28	120.64	117.00
1	AA	1410	A	N9-C4-C5	7.28	108.71	105.80
22	BA	2114	A	C4-C5-C6	7.28	120.64	117.00
22	BA	2225	A	C4-C5-C6	7.28	120.64	117.00
22	BA	1773	A	N9-C4-C5	7.27	108.71	105.80
22	BA	1966	A	C5-N7-C8	7.27	107.54	103.90
1	AA	1146	A	C5-N7-C8	7.27	107.54	103.90
1	AA	1476	A	C5-N7-C8	7.27	107.54	103.90
22	BA	160	A	C5-N7-C8	7.27	107.54	103.90
1	AA	19	A	C4-C5-C6	7.27	120.64	117.00
1	AA	864	A	C4-C5-C6	7.27	120.64	117.00
22	BA	42	A	N9-C4-C5	7.27	108.71	105.80
22	BA	1001	A	C5-N7-C8	7.27	107.53	103.90
22	BA	1269	A	C5-N7-C8	7.27	107.53	103.90
1	AA	1130	A	C5-N7-C8	7.27	107.53	103.90
22	BA	1580	A	C5-N7-C8	7.27	107.53	103.90
22	BA	1632	A	N9-C4-C5	7.27	108.71	105.80
23	BB	115	A	C5-N7-C8	7.27	107.53	103.90
22	BA	503	A	C4-C5-C6	7.27	120.63	117.00
22	BA	1336	A	C5-N7-C8	7.27	107.53	103.90
22	BA	2727	A	N3-C4-N9	7.27	133.21	127.40
1	AA	768	A	C4-C5-C6	7.26	120.63	117.00
1	AA	768	A	N9-C4-C5	7.26	108.70	105.80
22	BA	2776	A	N9-C4-C5	7.26	108.70	105.80
1	AA	964	A	C4-C5-C6	7.26	120.63	117.00
22	BA	556	A	C5-N7-C8	7.26	107.53	103.90
22	BA	1544	A	C5-N7-C8	7.26	107.53	103.90
22	BA	1098	A	C4-C5-C6	7.26	120.63	117.00
1	AA	1324	A	C4-C5-C6	7.25	120.63	117.00
1	AA	1437	A	C5-N7-C8	7.25	107.53	103.90
22	BA	311	A	C5-N7-C8	7.25	107.53	103.90
22	BA	675	A	N9-C4-C5	7.25	108.70	105.80
22	BA	1151	A	C5-N7-C8	7.25	107.53	103.90
22	BA	2412	A	C4-C5-C6	7.25	120.63	117.00
22	BA	2461	A	C4-C5-C6	7.25	120.63	117.00
22	BA	322	A	N9-C4-C5	7.25	108.70	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	677	A	C5-N7-C8	7.25	107.53	103.90
22	BA	1877	A	C5-N7-C8	7.25	107.53	103.90
22	BA	2070	A	N9-C4-C5	7.25	108.70	105.80
22	BA	2340	A	C5-N7-C8	7.25	107.53	103.90
22	BA	2542	A	C5-N7-C8	7.25	107.53	103.90
1	AA	282	A	C5-N7-C8	7.25	107.53	103.90
22	BA	241	A	C5-N7-C8	7.25	107.53	103.90
22	BA	1321	A	C5-N7-C8	7.25	107.53	103.90
22	BA	2705	A	C4-C5-C6	7.25	120.62	117.00
1	AA	609	A	C5-N7-C8	7.25	107.52	103.90
1	AA	509	A	C5-N7-C8	7.25	107.52	103.90
22	BA	1635	A	C4-C5-C6	7.25	120.62	117.00
22	BA	354	A	C5-N7-C8	7.25	107.52	103.90
1	AA	914	A	C5-N7-C8	7.24	107.52	103.90
22	BA	1103	A	C5-N7-C8	7.24	107.52	103.90
22	BA	1327	A	N9-C4-C5	7.24	108.70	105.80
22	BA	480	A	N9-C4-C5	7.24	108.70	105.80
22	BA	586	A	C4-C5-N7	-7.24	107.08	110.70
22	BA	2516	A	N9-C4-C5	7.24	108.70	105.80
1	AA	8	A	C5-N7-C8	7.24	107.52	103.90
1	AA	935	A	N9-C4-C5	7.24	108.69	105.80
22	BA	95	A	C4-C5-C6	7.24	120.62	117.00
22	BA	167	A	C4-C5-C6	7.24	120.62	117.00
22	BA	2432	A	C4-C5-C6	7.24	120.62	117.00
22	BA	1096	A	C5-N7-C8	7.24	107.52	103.90
22	BA	1276	A	C5-N7-C8	7.24	107.52	103.90
1	AA	768	A	C5-N7-C8	7.24	107.52	103.90
22	BA	309	A	N9-C4-C5	7.24	108.69	105.80
1	AA	913	A	C5-N7-C8	7.23	107.52	103.90
1	AA	1150	A	C5-N7-C8	7.23	107.52	103.90
22	BA	503	A	C5-N7-C8	7.23	107.52	103.90
22	BA	845	A	N3-C4-N9	7.23	133.19	127.40
1	AA	621	A	C5-N7-C8	7.23	107.52	103.90
1	AA	1000	A	C5-N7-C8	7.23	107.52	103.90
22	BA	794	A	N3-C4-N9	7.23	133.19	127.40
22	BA	1937	A	C4-C5-N7	-7.23	107.08	110.70
1	AA	675	A	N9-C4-C5	7.23	108.69	105.80
22	BA	472	A	C4-C5-C6	7.23	120.62	117.00
22	BA	2900	A	C4-C5-C6	7.23	120.62	117.00
1	AA	466	A	N9-C4-C5	7.23	108.69	105.80
22	BA	1969	A	C5-N7-C8	7.23	107.51	103.90
22	BA	2205	A	C5-N7-C8	7.23	107.51	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1105	A	C5-N7-C8	7.23	107.51	103.90
1	AA	1151	A	C5-N7-C8	7.23	107.51	103.90
1	AA	459	A	C4-C5-C6	7.22	120.61	117.00
22	BA	1127	A	C5-N7-C8	7.22	107.51	103.90
22	BA	2377	A	C5-N7-C8	7.22	107.51	103.90
1	AA	767	A	C5-N7-C8	7.22	107.51	103.90
22	BA	677	A	C4-C5-C6	7.22	120.61	117.00
22	BA	1669	A	N9-C4-C5	7.22	108.69	105.80
22	BA	2142	A	C5-N7-C8	7.22	107.51	103.90
22	BA	2459	A	C4-C5-C6	7.22	120.61	117.00
22	BA	38	A	N9-C4-C5	7.22	108.69	105.80
22	BA	282	A	C5-N7-C8	7.22	107.51	103.90
22	BA	1392	A	C5-N7-C8	7.22	107.51	103.90
1	AA	1110	A	C5-N7-C8	7.22	107.51	103.90
1	AA	1252	A	N9-C4-C5	7.22	108.69	105.80
1	AA	1413	A	C5-N7-C8	7.22	107.51	103.90
22	BA	1637	A	C4-C5-C6	7.22	120.61	117.00
22	BA	2646	C	C6-N1-C2	-7.22	117.41	120.30
22	BA	2809	A	C5-N7-C8	7.22	107.51	103.90
1	AA	994	A	C4-C5-C6	7.22	120.61	117.00
1	AA	1021	A	C5-N7-C8	7.22	107.51	103.90
1	AA	51	A	C5-N7-C8	7.22	107.51	103.90
1	AA	130	A	C5-N7-C8	7.22	107.51	103.90
1	AA	303	A	N9-C4-C5	7.22	108.69	105.80
55	B8	26	A	C5-N7-C8	7.22	107.51	103.90
1	AA	1261	A	C5-N7-C8	7.21	107.51	103.90
22	BA	735	A	C4-C5-C6	7.21	120.61	117.00
22	BA	2352	A	C4-C5-C6	7.21	120.61	117.00
1	AA	199	A	C5-N7-C8	7.21	107.51	103.90
1	AA	655	A	C4-C5-C6	7.21	120.61	117.00
1	AA	814	A	C4-C5-C6	7.21	120.61	117.00
1	AA	1311	A	N9-C4-C5	7.21	108.68	105.80
1	AA	1360	A	C4-C5-C6	7.21	120.61	117.00
1	AA	1483	A	C4-C5-C6	7.21	120.61	117.00
22	BA	572	A	N3-C4-N9	7.21	133.17	127.40
22	BA	899	A	N9-C4-C5	7.21	108.68	105.80
22	BA	2297	A	C4-C5-C6	7.21	120.61	117.00
22	BA	2736	A	N9-C4-C5	7.21	108.68	105.80
22	BA	2856	A	C5-N7-C8	7.21	107.50	103.90
22	BA	144	A	C5-N7-C8	7.21	107.50	103.90
22	BA	789	A	C5-N7-C8	7.21	107.50	103.90
22	BA	1204	A	N9-C4-C5	7.21	108.68	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	959	A	N9-C4-C5	7.21	108.68	105.80
1	AA	1201	A	C5-N7-C8	7.21	107.50	103.90
22	BA	2058	A	C5-N7-C8	7.21	107.50	103.90
22	BA	514	A	C5-N7-C8	7.21	107.50	103.90
22	BA	2461	A	C5-N7-C8	7.20	107.50	103.90
22	BA	1938	A	C4-C5-C6	7.20	120.60	117.00
1	AA	1269	A	N9-C4-C5	7.20	108.68	105.80
22	BA	44	A	C4-C5-C6	7.20	120.60	117.00
22	BA	1057	A	C5-N7-C8	7.20	107.50	103.90
22	BA	614	A	C5-N7-C8	7.20	107.50	103.90
22	BA	1749	A	C4-C5-C6	7.20	120.60	117.00
22	BA	2887	A	C5-N7-C8	7.20	107.50	103.90
22	BA	374	A	C5-N7-C8	7.20	107.50	103.90
22	BA	1010	A	N9-C4-C5	7.20	108.68	105.80
22	BA	1393	A	C5-N7-C8	7.20	107.50	103.90
22	BA	1552	A	C4-C5-C6	7.19	120.60	117.00
1	AA	161	A	C5-N7-C8	7.19	107.50	103.90
1	AA	1092	A	N9-C4-C5	7.19	108.68	105.80
22	BA	226	A	C5-N7-C8	7.19	107.50	103.90
1	AA	174	A	C5-N7-C8	7.19	107.50	103.90
1	AA	907	A	C5-N7-C8	7.19	107.50	103.90
22	BA	233	A	C5-N7-C8	7.19	107.50	103.90
22	BA	1616	A	C5-N7-C8	7.19	107.50	103.90
22	BA	654	A	C5-N7-C8	7.19	107.49	103.90
22	BA	342	A	C5-N7-C8	7.19	107.49	103.90
22	BA	1858	A	C5-N7-C8	7.19	107.49	103.90
1	AA	53	A	C5-N7-C8	7.18	107.49	103.90
1	AA	101	A	C4-C5-C6	7.18	120.59	117.00
22	BA	727	A	C5-N7-C8	7.18	107.49	103.90
1	AA	263	A	N9-C4-C5	7.18	108.67	105.80
22	BA	1439	A	N9-C4-C5	7.18	108.67	105.80
1	AA	149	A	C5-N7-C8	7.18	107.49	103.90
22	BA	182	A	C4-C5-C6	7.18	120.59	117.00
22	BA	346	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1998	A	N9-C4-C5	7.18	108.67	105.80
1	AA	1176	A	C4-C5-C6	7.18	120.59	117.00
1	AA	1179	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1054	A	C4-C5-C6	7.18	120.59	117.00
22	BA	1304	A	C5-N7-C8	7.18	107.49	103.90
1	AA	179	A	C5-N7-C8	7.17	107.49	103.90
1	AA	1035	A	C4-C5-C6	7.17	120.59	117.00
1	AA	1145	A	C5-N7-C8	7.17	107.49	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	497	A	C5-N7-C8	7.17	107.49	103.90
22	BA	661	A	C5-N7-C8	7.17	107.49	103.90
22	BA	928	A	C5-N7-C8	7.17	107.49	103.90
22	BA	1385	A	C5-N7-C8	7.17	107.49	103.90
22	BA	1913	A	C5-N7-C8	7.17	107.49	103.90
1	AA	1155	A	C5-N7-C8	7.17	107.48	103.90
1	AA	1157	A	C5-N7-C8	7.17	107.49	103.90
22	BA	1952	A	C5-N7-C8	7.17	107.48	103.90
22	BA	1301	A	N9-C4-C5	7.17	108.67	105.80
22	BA	2205	A	N9-C4-C5	7.17	108.67	105.80
22	BA	2212	A	N9-C4-C5	7.17	108.67	105.80
22	BA	2566	A	N3-C4-C5	-7.17	121.78	126.80
22	BA	2758	A	C5-N7-C8	7.17	107.48	103.90
1	AA	1014	A	C5-N7-C8	7.17	107.48	103.90
55	B8	20	U	O5'-P-OP1	7.17	119.30	110.70
22	BA	1156	A	C5-N7-C8	7.17	107.48	103.90
22	BA	1569	A	N9-C4-C5	7.17	108.67	105.80
1	AA	329	A	C4-C5-C6	7.16	120.58	117.00
1	AA	642	A	C4-C5-C6	7.16	120.58	117.00
1	AA	1246	A	N9-C4-C5	7.16	108.66	105.80
1	AA	81	A	C5-N7-C8	7.16	107.48	103.90
1	AA	315	A	C5-N7-C8	7.16	107.48	103.90
22	BA	513	A	N3-C4-N9	7.16	133.13	127.40
22	BA	2311	A	N9-C4-C5	7.16	108.66	105.80
22	BA	2726	A	C5-N7-C8	7.16	107.48	103.90
1	AA	1012	A	C4-C5-C6	7.16	120.58	117.00
1	AA	338	A	C4-C5-C6	7.16	120.58	117.00
1	AA	1102	A	C4-C5-C6	7.16	120.58	117.00
22	BA	2014	A	N9-C4-C5	7.16	108.66	105.80
1	AA	969	A	N9-C4-C5	7.15	108.66	105.80
55	B8	38	A	C8-N9-C4	7.15	108.66	105.80
1	AA	160	A	C5-N7-C8	7.15	107.47	103.90
22	BA	19	A	C5-N7-C8	7.15	107.47	103.90
23	BB	104	A	C5-N7-C8	7.15	107.47	103.90
1	AA	1408	A	C5-N7-C8	7.15	107.47	103.90
22	BA	1032	A	C5-N7-C8	7.15	107.47	103.90
1	AA	1456	A	C5-N7-C8	7.15	107.47	103.90
1	AA	1502	A	C5-N7-C8	7.15	107.47	103.90
22	BA	244	A	C5-N7-C8	7.15	107.47	103.90
22	BA	508	A	C5-N7-C8	7.15	107.47	103.90
22	BA	2598	A	C5-N7-C8	7.15	107.47	103.90
1	AA	1350	A	C5-N7-C8	7.15	107.47	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	344	A	C5-N7-C8	7.15	107.47	103.90
22	BA	2298	A	N9-C4-C5	7.15	108.66	105.80
22	BA	2346	A	C5-N7-C8	7.15	107.47	103.90
22	BA	2740	A	N9-C4-C5	7.15	108.66	105.80
1	AA	223	A	N9-C4-C5	7.14	108.66	105.80
1	AA	983	A	C5-N7-C8	7.14	107.47	103.90
22	BA	161	A	N9-C4-C5	7.14	108.66	105.80
22	BA	743	A	C5-N7-C8	7.14	107.47	103.90
1	AA	44	A	N9-C4-C5	7.14	108.66	105.80
1	AA	309	A	C5-N7-C8	7.14	107.47	103.90
1	AA	448	A	C5-N7-C8	7.14	107.47	103.90
1	AA	1248	A	C5-N7-C8	7.14	107.47	103.90
22	BA	182	A	C5-N7-C8	7.14	107.47	103.90
22	BA	478	A	C5-N7-C8	7.14	107.47	103.90
22	BA	2274	A	C5-N7-C8	7.14	107.47	103.90
22	BA	2860	A	C5-N7-C8	7.14	107.47	103.90
1	AA	1499	A	C5-N7-C8	7.14	107.47	103.90
1	AA	743	A	C5-N7-C8	7.14	107.47	103.90
1	AA	968	A	C5-N7-C8	7.14	107.47	103.90
22	BA	340	A	N9-C4-C5	7.14	108.66	105.80
22	BA	2900	A	C5-N7-C8	7.14	107.47	103.90
1	AA	98	A	C5-N7-C8	7.14	107.47	103.90
22	BA	2741	A	C5-N7-C8	7.14	107.47	103.90
1	AA	383	A	C5-N7-C8	7.14	107.47	103.90
1	AA	802	A	N9-C4-C5	7.14	108.65	105.80
1	AA	864	A	N9-C4-C5	7.14	108.66	105.80
1	AA	1022	A	N9-C4-C5	7.14	108.66	105.80
22	BA	2534	A	C5-N7-C8	7.13	107.47	103.90
22	BA	127	A	C5-N7-C8	7.13	107.47	103.90
22	BA	734	A	N9-C4-C5	7.13	108.65	105.80
22	BA	1919	A	C4-C5-C6	7.13	120.57	117.00
1	AA	749	A	C5-N7-C8	7.13	107.47	103.90
22	BA	2468	A	C5-N7-C8	7.13	107.47	103.90
1	AA	167	A	C5-N7-C8	7.13	107.46	103.90
1	AA	1044	A	N9-C4-C5	7.13	108.65	105.80
1	AA	1271	A	C5-N7-C8	7.13	107.46	103.90
22	BA	877	A	N9-C4-C5	7.13	108.65	105.80
22	BA	1077	A	C5-N7-C8	7.13	107.46	103.90
22	BA	1566	A	C5-N7-C8	7.13	107.46	103.90
22	BA	1848	A	C5-N7-C8	7.13	107.46	103.90
22	BA	1866	A	C4-C5-C6	7.13	120.56	117.00
1	AA	959	A	C4-C5-C6	7.13	120.56	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1492	A	C5-N7-C8	7.13	107.46	103.90
22	BA	42	A	C5-N7-C8	7.13	107.46	103.90
22	BA	2059	A	C5-N7-C8	7.13	107.46	103.90
1	AA	499	A	C4-C5-C6	7.12	120.56	117.00
22	BA	1080	A	C4-C5-C6	7.12	120.56	117.00
1	AA	353	A	N9-C4-C5	7.12	108.65	105.80
1	AA	696	A	C4-C5-C6	7.12	120.56	117.00
1	AA	946	A	C5-N7-C8	7.12	107.46	103.90
22	BA	2211	A	N9-C4-C5	7.12	108.65	105.80
1	AA	554	A	C5-N7-C8	7.12	107.46	103.90
22	BA	2700	A	C4-C5-C6	7.12	120.56	117.00
1	AA	694	A	N9-C4-C5	7.12	108.65	105.80
22	BA	1717	A	C5-N7-C8	7.12	107.46	103.90
23	BB	53	A	N9-C4-C5	7.12	108.65	105.80
1	AA	630	A	C5-N7-C8	7.12	107.46	103.90
1	AA	964	A	N9-C4-C5	7.12	108.65	105.80
22	BA	1532	A	C5-N7-C8	7.12	107.46	103.90
1	AA	327	A	C5-N7-C8	7.11	107.46	103.90
1	AA	1055	A	C5-N7-C8	7.11	107.46	103.90
22	BA	1143	A	C4-C5-C6	7.11	120.56	117.00
22	BA	1395	A	N9-C4-C5	7.11	108.65	105.80
22	BA	1427	A	N9-C4-C5	7.11	108.64	105.80
22	BA	1549	A	C5-N7-C8	7.11	107.46	103.90
22	BA	1918	A	C5-N7-C8	7.11	107.46	103.90
22	BA	2530	A	C5-N7-C8	7.11	107.46	103.90
22	BA	2600	A	C4-C5-C6	7.11	120.56	117.00
22	BA	1593	A	C5-N7-C8	7.11	107.46	103.90
22	BA	2513	A	C4-C5-C6	7.11	120.56	117.00
22	BA	2879	A	C4-C5-C6	7.11	120.56	117.00
1	AA	1171	A	C5-N7-C8	7.11	107.45	103.90
22	BA	2899	A	C5-N7-C8	7.11	107.46	103.90
22	BA	227	A	C5-N7-C8	7.11	107.45	103.90
1	AA	1019	A	N9-C4-C5	7.11	108.64	105.80
22	BA	910	A	C5-N7-C8	7.11	107.45	103.90
1	AA	547	A	N9-C4-C5	7.11	108.64	105.80
1	AA	1350	A	C4-C5-C6	7.11	120.55	117.00
22	BA	1103	A	C4-C5-C6	7.11	120.55	117.00
22	BA	362	A	C4-C5-C6	7.10	120.55	117.00
22	BA	1264	A	N9-C4-C5	7.10	108.64	105.80
1	AA	238	A	N9-C4-C5	7.10	108.64	105.80
1	AA	344	A	C5-N7-C8	7.10	107.45	103.90
1	AA	563	A	N3-C4-N9	7.10	133.08	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1152	A	C4-C5-C6	7.10	120.55	117.00
23	BB	45	A	C4-C5-C6	7.10	120.55	117.00
22	BA	1095	A	C4-C5-C6	7.10	120.55	117.00
22	BA	1413	A	C4-C5-C6	7.10	120.55	117.00
1	AA	190	A	C5-N7-C8	7.10	107.45	103.90
1	AA	1046	A	N3-C4-N9	7.10	133.08	127.40
22	BA	1039	A	C5-N7-C8	7.10	107.45	103.90
23	BB	115	A	N9-C4-C5	7.10	108.64	105.80
22	BA	917	A	C4-C5-C6	7.10	120.55	117.00
1	AA	243	A	N9-C4-C5	7.09	108.64	105.80
1	AA	1346	A	C5-N7-C8	7.09	107.45	103.90
22	BA	56	A	C5-N7-C8	7.09	107.45	103.90
22	BA	1427	A	C5-N7-C8	7.09	107.45	103.90
22	BA	1571	A	C5-N7-C8	7.09	107.45	103.90
1	AA	502	A	C5-N7-C8	7.09	107.45	103.90
22	BA	1522	A	C5-N7-C8	7.09	107.45	103.90
1	AA	393	A	C5-N7-C8	7.09	107.45	103.90
22	BA	1571	A	C4-C5-C6	7.09	120.55	117.00
22	BA	1848	A	C5-C6-N1	7.09	121.25	117.70
22	BA	1021	A	N3-C4-N9	7.09	133.07	127.40
22	BA	1142	A	C5-N7-C8	7.09	107.44	103.90
22	BA	705	A	N3-C4-N9	7.09	133.07	127.40
22	BA	13	A	C4-C5-N7	-7.09	107.16	110.70
22	BA	590	A	C5-N7-C8	7.09	107.44	103.90
22	BA	602	A	C5-N7-C8	7.09	107.44	103.90
22	BA	1711	A	C5-N7-C8	7.09	107.44	103.90
1	AA	831	A	C5-N7-C8	7.08	107.44	103.90
1	AA	816	A	C5-N7-C8	7.08	107.44	103.90
22	BA	1808	A	N9-C4-C5	7.08	108.63	105.80
1	AA	487	A	C5-N7-C8	7.08	107.44	103.90
22	BA	196	A	C4-C5-C6	7.08	120.54	117.00
22	BA	447	A	C5-N7-C8	7.08	107.44	103.90
22	BA	896	A	C5-N7-C8	7.08	107.44	103.90
22	BA	1098	A	C5-N7-C8	7.08	107.44	103.90
1	AA	1329	A	N9-C4-C5	7.08	108.63	105.80
22	BA	981	A	C5-N7-C8	7.08	107.44	103.90
22	BA	1165	A	C5-N7-C8	7.08	107.44	103.90
1	AA	456	A	C5-N7-C8	7.08	107.44	103.90
1	AA	635	A	C5-N7-C8	7.08	107.44	103.90
1	AA	790	A	C5-N7-C8	7.08	107.44	103.90
1	AA	1289	A	C5-N7-C8	7.08	107.44	103.90
22	BA	1254	A	C5-N7-C8	7.08	107.44	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2003	A	N9-C4-C5	7.08	108.63	105.80
23	BB	73	A	C5-N7-C8	7.08	107.44	103.90
22	BA	1755	A	N9-C4-C5	7.07	108.63	105.80
22	BA	2823	A	C5-N7-C8	7.07	107.44	103.90
1	AA	482	A	N9-C4-C5	7.07	108.63	105.80
1	AA	1456	A	N9-C4-C5	7.07	108.63	105.80
22	BA	979	A	C5-N7-C8	7.07	107.44	103.90
22	BA	1665	A	C5-N7-C8	7.07	107.44	103.90
22	BA	1802	A	C4-C5-C6	7.07	120.54	117.00
1	AA	197	A	N9-C4-C5	7.07	108.63	105.80
22	BA	933	A	C5-N7-C8	7.07	107.44	103.90
22	BA	984	A	N9-C4-C5	7.07	108.63	105.80
22	BA	2090	A	C5-N7-C8	7.07	107.44	103.90
22	BA	2335	A	N9-C4-C5	7.07	108.63	105.80
22	BA	761	A	C4-C5-C6	7.07	120.53	117.00
1	AA	937	A	C5-N7-C8	7.07	107.43	103.90
22	BA	1244	A	N3-C4-N9	7.07	133.05	127.40
1	AA	263	A	C5-N7-C8	7.07	107.43	103.90
1	AA	382	A	C4-C5-C6	7.07	120.53	117.00
1	AA	539	A	C4-C5-C6	7.07	120.53	117.00
1	AA	907	A	C4-C5-C6	7.07	120.53	117.00
22	BA	384	A	C5-N7-C8	7.07	107.43	103.90
22	BA	1095	A	C5-N7-C8	7.07	107.43	103.90
22	BA	1395	A	C5-N7-C8	7.07	107.43	103.90
22	BA	2675	A	C5-N7-C8	7.07	107.43	103.90
22	BA	1773	A	C4-C5-C6	7.06	120.53	117.00
22	BA	1872	A	C5-N7-C8	7.06	107.43	103.90
22	BA	1970	A	O5'-P-OP2	7.06	119.18	110.70
1	AA	1117	A	C5-N7-C8	7.06	107.43	103.90
1	AA	1196	A	C5-N7-C8	7.06	107.43	103.90
22	BA	1698	A	C5-N7-C8	7.06	107.43	103.90
22	BA	2211	A	C5-N7-C8	7.06	107.43	103.90
1	AA	1092	A	C5-N7-C8	7.06	107.43	103.90
22	BA	330	A	C5-N7-C8	7.06	107.43	103.90
22	BA	1050	A	N9-C4-C5	7.06	108.62	105.80
22	BA	1938	A	C5-N7-C8	7.06	107.43	103.90
22	BA	1953	A	C5-N7-C8	7.06	107.43	103.90
1	AA	414	A	N9-C4-C5	7.06	108.62	105.80
22	BA	460	A	C5-N7-C8	7.06	107.43	103.90
22	BA	1701	A	N9-C4-C5	7.06	108.62	105.80
22	BA	1960	A	N9-C4-C5	7.06	108.62	105.80
1	AA	171	A	C5-N7-C8	7.06	107.43	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1252	A	C4-C5-C6	7.06	120.53	117.00
22	BA	94	A	N9-C4-C5	7.06	108.62	105.80
22	BA	2013	A	C5-N7-C8	7.06	107.43	103.90
22	BA	2071	A	C4-C5-C6	7.06	120.53	117.00
1	AA	270	A	C4-C5-C6	7.05	120.53	117.00
1	AA	816	A	N9-C4-C5	7.05	108.62	105.80
22	BA	1503	A	C5-N7-C8	7.05	107.43	103.90
1	AA	767	A	C4-C5-C6	7.05	120.53	117.00
1	AA	1285	A	C5-N7-C8	7.05	107.43	103.90
22	BA	141	G	N9-C4-C5	-7.05	102.58	105.40
22	BA	1431	A	N9-C4-C5	7.05	108.62	105.80
22	BA	1635	A	C5-N7-C8	7.05	107.42	103.90
1	AA	766	A	C5-N7-C8	7.05	107.42	103.90
1	AA	819	A	C5-N7-C8	7.05	107.42	103.90
22	BA	309	A	C5-N7-C8	7.05	107.42	103.90
22	BA	2117	A	C5-N7-C8	7.05	107.42	103.90
22	BA	204	A	N9-C4-C5	7.05	108.62	105.80
1	AA	81	A	N9-C4-C5	7.05	108.62	105.80
22	BA	1413	A	N9-C4-C5	7.04	108.62	105.80
22	BA	522	A	C5-N7-C8	7.04	107.42	103.90
22	BA	1739	A	N9-C4-C5	7.04	108.62	105.80
1	AA	205	A	C4-C5-C6	7.04	120.52	117.00
1	AA	728	A	C5-N7-C8	7.04	107.42	103.90
1	AA	1429	A	C4-C5-C6	7.04	120.52	117.00
55	B8	59	A	C4-C5-C6	7.04	120.52	117.00
1	AA	782	A	C5-N7-C8	7.04	107.42	103.90
22	BA	104	A	C4-C5-C6	7.04	120.52	117.00
22	BA	637	A	C5-N7-C8	7.04	107.42	103.90
22	BA	1508	A	C5-N7-C8	7.04	107.42	103.90
1	AA	393	A	N9-C4-C5	7.04	108.61	105.80
1	AA	1468	A	C5-N7-C8	7.04	107.42	103.90
22	BA	590	A	C4-C5-C6	7.04	120.52	117.00
1	AA	977	A	C5-N7-C8	7.03	107.42	103.90
22	BA	878	A	C5-N7-C8	7.03	107.42	103.90
22	BA	1008	A	C5-N7-C8	7.03	107.42	103.90
22	BA	2052	A	C5-N7-C8	7.03	107.42	103.90
22	BA	2886	A	C5-N7-C8	7.03	107.42	103.90
1	AA	364	A	N9-C4-C5	7.03	108.61	105.80
22	BA	1262	A	C4-C5-C6	7.03	120.52	117.00
1	AA	366	A	C4-C5-C6	7.03	120.52	117.00
1	AA	459	A	N3-C4-N9	7.03	133.03	127.40
1	AA	1377	A	N9-C4-C5	7.03	108.61	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	513	A	C5-N7-C8	7.03	107.42	103.90
22	BA	1654	A	C5-N7-C8	7.03	107.42	103.90
22	BA	2071	A	N9-C4-C5	7.03	108.61	105.80
22	BA	2392	A	C5-N7-C8	7.03	107.42	103.90
1	AA	1333	A	N9-C4-C5	7.03	108.61	105.80
1	AA	10	A	C5-N7-C8	7.03	107.41	103.90
1	AA	415	A	C5-N7-C8	7.03	107.41	103.90
22	BA	613	A	C4-C5-C6	7.03	120.51	117.00
22	BA	1918	A	C4-C5-C6	7.03	120.51	117.00
1	AA	1102	A	C5-N7-C8	7.03	107.41	103.90
22	BA	125	A	N9-C4-C5	7.03	108.61	105.80
22	BA	1609	A	C5-N7-C8	7.03	107.41	103.90
22	BA	2205	A	C4-C5-C6	7.03	120.51	117.00
22	BA	2327	A	N9-C4-C5	7.03	108.61	105.80
22	BA	2425	A	C4-C5-C6	7.03	120.51	117.00
22	BA	863	A	C5-N7-C8	7.02	107.41	103.90
22	BA	975	A	C4-C5-N7	-7.02	107.19	110.70
1	AA	139	A	C5-N7-C8	7.02	107.41	103.90
1	AA	1093	A	C5-N7-C8	7.02	107.41	103.90
22	BA	104	A	N9-C4-C5	7.02	108.61	105.80
22	BA	609	A	C5-N7-C8	7.02	107.41	103.90
22	BA	689	A	N9-C4-C5	7.02	108.61	105.80
22	BA	1144	A	N9-C4-C5	7.02	108.61	105.80
22	BA	1040	A	C5-N7-C8	7.02	107.41	103.90
22	BA	2284	A	C5-N7-C8	7.02	107.41	103.90
1	AA	815	A	N9-C4-C5	7.02	108.61	105.80
22	BA	1254	A	N9-C4-C5	7.02	108.61	105.80
22	BA	2531	A	C4-C5-C6	7.02	120.51	117.00
22	BA	219	A	C5-N7-C8	7.02	107.41	103.90
22	BA	1129	A	C5-N7-C8	7.02	107.41	103.90
22	BA	2019	A	C4-C5-C6	7.02	120.51	117.00
22	BA	1134	A	C4-C5-C6	7.02	120.51	117.00
22	BA	2572	A	C8-N9-C4	7.02	108.61	105.80
1	AA	364	A	C5-N7-C8	7.01	107.41	103.90
22	BA	541	A	N9-C4-C5	7.01	108.61	105.80
22	BA	716	A	C5-N7-C8	7.01	107.41	103.90
22	BA	936	A	C5-N7-C8	7.01	107.41	103.90
22	BA	2899	A	N9-C4-C5	7.01	108.61	105.80
22	BA	2058	A	C4-C5-C6	7.01	120.51	117.00
1	AA	1191	A	C4-C5-C6	7.01	120.51	117.00
22	BA	439	A	C5-N7-C8	7.01	107.41	103.90
22	BA	909	A	C5-N7-C8	7.01	107.41	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1819	A	C4-C5-C6	7.01	120.51	117.00
1	AA	1534	A	N9-C4-C5	7.01	108.60	105.80
22	BA	2288	A	C4-C5-C6	7.01	120.50	117.00
1	AA	411	A	C5-N7-C8	7.01	107.40	103.90
22	BA	1111	A	C4-C5-C6	7.01	120.50	117.00
22	BA	1579	A	C5-N7-C8	7.01	107.40	103.90
22	BA	1722	A	C5-N7-C8	7.01	107.40	103.90
22	BA	2829	A	C5-N7-C8	7.01	107.40	103.90
1	AA	782	A	N9-C4-C5	7.00	108.60	105.80
1	AA	878	A	C5-N7-C8	7.00	107.40	103.90
22	BA	402	A	C5-N7-C8	7.00	107.40	103.90
22	BA	1569	A	C5-N7-C8	7.00	107.40	103.90
22	BA	1650	A	C5-N7-C8	7.00	107.40	103.90
22	BA	2147	A	N9-C4-C5	7.00	108.60	105.80
22	BA	2639	A	C5-N7-C8	7.00	107.40	103.90
55	B8	14	A	C4-C5-C6	7.00	120.50	117.00
22	BA	95	A	C5-N7-C8	7.00	107.40	103.90
22	BA	721	A	C5-N7-C8	7.00	107.40	103.90
22	BA	783	A	C4-C5-C6	7.00	120.50	117.00
22	BA	2577	A	C4-C5-N7	-7.00	107.20	110.70
1	AA	889	A	C5-N7-C8	7.00	107.40	103.90
1	AA	974	A	C5-N7-C8	7.00	107.40	103.90
22	BA	616	A	C4-C5-C6	7.00	120.50	117.00
22	BA	1367	A	C5-N7-C8	7.00	107.40	103.90
1	AA	1480	A	C5-N7-C8	7.00	107.40	103.90
22	BA	2366	A	C4-C5-C6	7.00	120.50	117.00
1	AA	1250	A	C5-N7-C8	7.00	107.40	103.90
22	BA	863	A	N3-C4-N9	6.99	132.99	127.40
1	AA	780	A	C5-N7-C8	6.99	107.40	103.90
22	BA	466	A	C5-N7-C8	6.99	107.40	103.90
22	BA	2309	A	N9-C4-C5	6.99	108.60	105.80
22	BA	2426	A	C5-N7-C8	6.99	107.40	103.90
1	AA	282	A	N9-C4-C5	6.99	108.60	105.80
22	BA	730	A	C5-C6-N6	6.99	129.29	123.70
1	AA	1434	A	C4-C5-C6	6.99	120.49	117.00
22	BA	918	A	C5-N7-C8	6.99	107.39	103.90
22	BA	2051	A	C5-N7-C8	6.99	107.39	103.90
22	BA	2800	A	C5-N7-C8	6.99	107.39	103.90
1	AA	274	A	C5-N7-C8	6.99	107.39	103.90
1	AA	595	A	C5-N7-C8	6.99	107.39	103.90
22	BA	1268	A	C5-N7-C8	6.99	107.39	103.90
22	BA	502	A	C5-N7-C8	6.98	107.39	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2453	A	N9-C4-C5	6.98	108.59	105.80
1	AA	1102	A	N9-C4-C5	6.98	108.59	105.80
1	AA	1250	A	N9-C4-C5	6.98	108.59	105.80
22	BA	294	A	C5-N7-C8	6.98	107.39	103.90
22	BA	613	A	C5-N7-C8	6.98	107.39	103.90
1	AA	253	A	C5-N7-C8	6.98	107.39	103.90
1	AA	573	A	C5-N7-C8	6.98	107.39	103.90
1	AA	1339	A	C4-C5-C6	6.98	120.49	117.00
22	BA	2154	A	C4-C5-C6	6.98	120.49	117.00
22	BA	2738	A	C5-N7-C8	6.98	107.39	103.90
22	BA	49	A	C5-N7-C8	6.98	107.39	103.90
1	AA	807	A	C5-N7-C8	6.98	107.39	103.90
22	BA	149	A	C5-N7-C8	6.98	107.39	103.90
22	BA	368	A	C5-N7-C8	6.98	107.39	103.90
22	BA	538	A	C5-N7-C8	6.98	107.39	103.90
22	BA	781	A	C4-C5-N7	-6.98	107.21	110.70
22	BA	2741	A	C4-C5-C6	6.98	120.49	117.00
22	BA	980	A	C4-C5-C6	6.97	120.49	117.00
22	BA	1821	A	N9-C4-C5	6.97	108.59	105.80
1	AA	759	A	C5-N7-C8	6.97	107.39	103.90
22	BA	5	A	C4-C5-C6	6.97	120.49	117.00
22	BA	127	A	N9-C4-C5	6.97	108.59	105.80
22	BA	1378	A	C5-N7-C8	6.97	107.39	103.90
22	BA	1590	A	C5-N7-C8	6.97	107.39	103.90
22	BA	2810	A	C5-N7-C8	6.97	107.39	103.90
1	AA	1362	A	C5-N7-C8	6.97	107.38	103.90
22	BA	909	A	N9-C4-C5	6.97	108.59	105.80
22	BA	1545	A	C5-N7-C8	6.97	107.39	103.90
22	BA	1977	A	C5-N7-C8	6.97	107.38	103.90
22	BA	2173	A	C4-C5-C6	6.97	120.48	117.00
1	AA	509	A	C4-C5-C6	6.97	120.48	117.00
1	AA	681	A	C5-N7-C8	6.97	107.38	103.90
1	AA	1101	A	N9-C4-C5	6.97	108.59	105.80
22	BA	348	A	C5-N7-C8	6.97	107.38	103.90
22	BA	453	A	C5-N7-C8	6.97	107.38	103.90
22	BA	1552	A	N9-C4-C5	6.97	108.59	105.80
1	AA	535	A	C5-N7-C8	6.96	107.38	103.90
22	BA	131	A	C5-N7-C8	6.96	107.38	103.90
22	BA	1301	A	C5-N7-C8	6.96	107.38	103.90
22	BA	1580	A	C4-C5-C6	6.96	120.48	117.00
22	BA	1810	A	C5-N7-C8	6.96	107.38	103.90
1	AA	298	A	C5-N7-C8	6.96	107.38	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1705	A	C5-N7-C8	6.96	107.38	103.90
1	AA	860	A	C4-C5-N7	-6.96	107.22	110.70
1	AA	878	A	N9-C4-C5	6.96	108.58	105.80
22	BA	324	A	C5-N7-C8	6.96	107.38	103.90
22	BA	715	A	C5-N7-C8	6.96	107.38	103.90
1	AA	66	A	C5-N7-C8	6.96	107.38	103.90
22	BA	374	A	C4-C5-C6	6.96	120.48	117.00
22	BA	752	A	C4-C5-N7	-6.96	107.22	110.70
22	BA	1307	A	C4-C5-C6	6.96	120.48	117.00
22	BA	2169	A	C5-N7-C8	6.96	107.38	103.90
1	AA	143	A	N9-C4-C5	6.96	108.58	105.80
1	AA	192	A	C5-N7-C8	6.96	107.38	103.90
1	AA	1447	A	C5-N7-C8	6.96	107.38	103.90
22	BA	1735	A	C5-N7-C8	6.96	107.38	103.90
1	AA	303	A	C5-N7-C8	6.96	107.38	103.90
1	AA	1188	A	C5-N7-C8	6.96	107.38	103.90
1	AA	1201	A	N3-C4-N9	6.96	132.96	127.40
22	BA	332	A	C5-N7-C8	6.96	107.38	103.90
22	BA	603	A	C5-N7-C8	6.96	107.38	103.90
1	AA	482	A	C5-N7-C8	6.95	107.38	103.90
1	AA	753	A	C5-N7-C8	6.95	107.38	103.90
22	BA	526	A	C5-N7-C8	6.95	107.38	103.90
22	BA	2665	A	C4-C5-C6	6.95	120.48	117.00
2	AB	205	ASP	N-CA-CB	-6.95	98.09	110.60
22	BA	1383	A	C5-N7-C8	6.95	107.38	103.90
22	BA	1614	A	C4-C5-C6	6.95	120.48	117.00
1	AA	274	A	C5-C6-N1	6.95	121.17	117.70
22	BA	1916	A	C4-C5-C6	6.95	120.47	117.00
22	BA	2169	A	N9-C4-C5	6.95	108.58	105.80
22	BA	94	A	C4-C5-C6	6.95	120.47	117.00
22	BA	1307	A	N9-C4-C5	6.95	108.58	105.80
22	BA	1453	A	N9-C4-C5	6.95	108.58	105.80
22	BA	2679	A	C4-C5-C6	6.95	120.47	117.00
1	AA	1012	A	C5-N7-C8	6.95	107.37	103.90
22	BA	14	A	N9-C4-C5	6.95	108.58	105.80
22	BA	299	A	C5-N7-C8	6.95	107.37	103.90
22	BA	2450	A	C5-N7-C8	6.95	107.37	103.90
1	AA	1394	A	C5-N7-C8	6.94	107.37	103.90
22	BA	2183	A	C5-N7-C8	6.94	107.37	103.90
1	AA	595	A	N9-C4-C5	6.94	108.58	105.80
22	BA	2033	A	C4-C5-N7	-6.94	107.23	110.70
1	AA	539	A	N9-C4-C5	6.94	108.58	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	629	A	C4-C5-C6	6.94	120.47	117.00
22	BA	173	A	C5-N7-C8	6.94	107.37	103.90
22	BA	354	A	N9-C4-C5	6.94	108.58	105.80
22	BA	2095	A	C4-C5-C6	6.94	120.47	117.00
22	BA	2171	A	C5-N7-C8	6.94	107.37	103.90
22	BA	2814	A	C4-C5-C6	6.94	120.47	117.00
1	AA	502	A	N9-C4-C5	6.94	108.58	105.80
22	BA	2750	A	C5-N7-C8	6.94	107.37	103.90
1	AA	32	A	C5-N7-C8	6.94	107.37	103.90
1	AA	974	A	N9-C4-C5	6.94	108.58	105.80
1	AA	1	A	C4-C5-C6	6.94	120.47	117.00
1	AA	1216	A	C5-N7-C8	6.94	107.37	103.90
22	BA	1762	A	C5-N7-C8	6.94	107.37	103.90
22	BA	344	A	C4-C5-C6	6.93	120.47	117.00
22	BA	1434	A	C4-C5-N7	-6.93	107.23	110.70
22	BA	1572	A	C5-N7-C8	6.93	107.37	103.90
1	AA	366	A	C5-N7-C8	6.93	107.37	103.90
22	BA	2813	A	C4-C5-C6	6.93	120.47	117.00
1	AA	192	A	N9-C4-C5	6.93	108.57	105.80
1	AA	825	A	N9-C4-C5	6.93	108.57	105.80
22	BA	64	A	C5-N7-C8	6.93	107.37	103.90
22	BA	2534	A	C4-C5-C6	6.93	120.47	117.00
1	AA	900	A	N9-C4-C5	6.93	108.57	105.80
22	BA	278	A	C4-C5-C6	6.93	120.46	117.00
22	BA	718	A	C4-C5-C6	6.93	120.46	117.00
22	BA	1313	U	C2-N1-C1'	6.93	126.01	117.70
1	AA	1044	A	C5-N7-C8	6.93	107.36	103.90
22	BA	1020	A	N9-C4-C5	6.93	108.57	105.80
22	BA	1553	A	C5-N7-C8	6.93	107.36	103.90
1	AA	65	A	C5-N7-C8	6.92	107.36	103.90
22	BA	2358	A	N9-C4-C5	6.92	108.57	105.80
22	BA	2322	A	C5-N7-C8	6.92	107.36	103.90
22	BA	347	A	N9-C4-C5	6.92	108.57	105.80
22	BA	800	A	C4-C5-N7	-6.92	107.24	110.70
1	AA	533	A	N3-C4-N9	6.92	132.94	127.40
1	AA	1145	A	N9-C4-C5	6.92	108.57	105.80
1	AA	1363	A	C5-N7-C8	6.92	107.36	103.90
1	AA	1430	A	N9-C4-C5	6.92	108.57	105.80
22	BA	1899	A	N9-C4-C5	6.92	108.57	105.80
22	BA	2119	A	N9-C4-C5	6.92	108.57	105.80
22	BA	2352	A	N9-C4-C5	6.92	108.57	105.80
22	BA	199	A	C5-N7-C8	6.92	107.36	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	155	A	C5-N7-C8	6.92	107.36	103.90
1	AA	238	A	C5-N7-C8	6.92	107.36	103.90
22	BA	38	A	C4-C5-C6	6.92	120.46	117.00
22	BA	1020	A	C5-N7-C8	6.92	107.36	103.90
22	BA	2587	A	C5-C6-N1	6.92	121.16	117.70
22	BA	2721	A	C4-C5-C6	6.92	120.46	117.00
22	BA	1010	A	C5-N7-C8	6.91	107.36	103.90
22	BA	1073	A	C4-C5-C6	6.91	120.46	117.00
22	BA	2660	A	C5-N7-C8	6.91	107.36	103.90
1	AA	325	A	C5-N7-C8	6.91	107.35	103.90
22	BA	103	A	C4-C5-C6	6.91	120.45	117.00
22	BA	1678	A	N9-C4-C5	6.91	108.56	105.80
22	BA	1998	A	C4-C5-C6	6.91	120.45	117.00
22	BA	2281	A	C4-C5-C6	6.91	120.45	117.00
1	AA	119	A	C5-N7-C8	6.91	107.35	103.90
1	AA	938	A	N9-C4-C5	6.91	108.56	105.80
22	BA	532	A	C4-C5-C6	6.91	120.45	117.00
22	BA	2376	A	C5-N7-C8	6.91	107.35	103.90
1	AA	946	A	C4-C5-C6	6.91	120.45	117.00
22	BA	2675	A	C4-C5-C6	6.91	120.45	117.00
22	BA	2829	A	N9-C4-C5	6.91	108.56	105.80
1	AA	520	A	C4-C5-C6	6.90	120.45	117.00
22	BA	1494	A	C4-C5-C6	6.90	120.45	117.00
22	BA	541	A	C5-N7-C8	6.90	107.35	103.90
1	AA	749	A	N9-C4-C5	6.90	108.56	105.80
1	AA	1493	A	C5-N7-C8	6.90	107.35	103.90
22	BA	352	A	C5-N7-C8	6.90	107.35	103.90
22	BA	2476	A	N9-C4-C5	6.90	108.56	105.80
1	AA	262	A	C5-N7-C8	6.90	107.35	103.90
1	AA	495	A	C5-N7-C8	6.90	107.35	103.90
22	BA	382	A	C5-N7-C8	6.90	107.35	103.90
22	BA	2900	A	N9-C4-C5	6.90	108.56	105.80
1	AA	1408	A	C4-C5-C6	6.90	120.45	117.00
22	BA	142	A	C4-C5-C6	6.90	120.45	117.00
1	AA	649	A	C5-N7-C8	6.90	107.35	103.90
1	AA	3	A	N9-C4-C5	6.89	108.56	105.80
22	BA	833	A	N9-C4-C5	6.89	108.56	105.80
22	BA	1570	A	N9-C4-C5	6.89	108.56	105.80
22	BA	2274	A	C4-C5-C6	6.89	120.45	117.00
22	BA	2406	A	C5-N7-C8	6.89	107.35	103.90
1	AA	712	A	C4-C5-C6	6.89	120.45	117.00
22	BA	73	A	C5-N7-C8	6.89	107.35	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	144	A	C4-C5-C6	6.89	120.45	117.00
22	BA	197	A	C4-C5-C6	6.89	120.45	117.00
1	AA	1491	G	C8-N9-C4	6.89	109.16	106.40
22	BA	1144	A	C4-C5-C6	6.89	120.44	117.00
1	AA	1042	A	C5-N7-C8	6.89	107.34	103.90
22	BA	1365	A	C4-C5-C6	6.89	120.44	117.00
22	BA	1635	A	N9-C4-C5	6.89	108.56	105.80
22	BA	119	A	C5-N7-C8	6.89	107.34	103.90
22	BA	330	A	N3-C4-N9	6.89	132.91	127.40
22	BA	582	A	C4-C5-C6	6.89	120.44	117.00
1	AA	553	A	N9-C4-C5	6.88	108.55	105.80
1	AA	1429	A	N9-C4-C5	6.88	108.55	105.80
22	BA	265	A	C5-N7-C8	6.88	107.34	103.90
22	BA	2284	A	N3-C4-N9	6.88	132.91	127.40
1	AA	33	A	C5-N7-C8	6.88	107.34	103.90
22	BA	2850	A	C4-C5-C6	6.88	120.44	117.00
22	BA	482	A	C5-N7-C8	6.88	107.34	103.90
22	BA	699	A	C4-C5-N7	-6.88	107.26	110.70
1	AA	609	A	N9-C4-C5	6.88	108.55	105.80
1	AA	1257	A	C5-N7-C8	6.88	107.34	103.90
22	BA	1583	A	N9-C4-C5	6.88	108.55	105.80
1	AA	964	A	C5-N7-C8	6.88	107.34	103.90
22	BA	1084	A	N9-C4-C5	6.88	108.55	105.80
1	AA	621	A	C4-C5-C6	6.88	120.44	117.00
1	AA	1306	A	C5-N7-C8	6.88	107.34	103.90
22	BA	384	A	C4-C5-C6	6.88	120.44	117.00
22	BA	472	A	C5-N7-C8	6.88	107.34	103.90
22	BA	1664	A	C5-N7-C8	6.88	107.34	103.90
22	BA	2090	A	C4-C5-C6	6.88	120.44	117.00
22	BA	2199	A	N9-C4-C5	6.88	108.55	105.80
1	AA	1368	A	C4-C5-C6	6.88	120.44	117.00
22	BA	471	A	C5-N7-C8	6.88	107.34	103.90
1	AA	441	A	C4-C5-C6	6.87	120.44	117.00
1	AA	901	A	N3-C4-N9	6.87	132.90	127.40
22	BA	945	A	C5-N7-C8	6.87	107.34	103.90
22	BA	1672	A	N9-C4-C5	6.87	108.55	105.80
22	BA	2270	A	C4-C5-C6	6.87	120.44	117.00
1	AA	975	A	C5-N7-C8	6.87	107.33	103.90
1	AA	1201	A	C5-C6-N6	6.87	129.20	123.70
1	AA	1320	C	O5'-P-OP2	6.87	118.95	110.70
22	BA	599	A	C5-N7-C8	6.87	107.34	103.90
1	AA	49	U	N3-C4-O4	-6.87	114.59	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1289	A	N9-C4-C5	6.87	108.55	105.80
22	BA	2267	A	N3-C4-N9	6.87	132.90	127.40
23	BB	45	A	C5-N7-C8	6.87	107.33	103.90
1	AA	1271	A	C4-C5-C6	6.87	120.43	117.00
1	AA	1363	A	C4-C5-C6	6.87	120.44	117.00
22	BA	423	A	C4-C5-C6	6.87	120.43	117.00
22	BA	2170	A	C5-N7-C8	6.87	107.33	103.90
22	BA	368	A	C4-C5-C6	6.87	120.43	117.00
1	AA	695	A	C4-C5-C6	6.86	120.43	117.00
22	BA	1637	A	N9-C4-C5	6.86	108.55	105.80
1	AA	1483	A	C5-N7-C8	6.86	107.33	103.90
22	BA	1502	A	C5-N7-C8	6.86	107.33	103.90
1	AA	3	A	C5-N7-C8	6.86	107.33	103.90
22	BA	943	A	C5-N7-C8	6.86	107.33	103.90
22	BA	1384	A	C5-N7-C8	6.86	107.33	103.90
23	BB	78	A	N9-C4-C5	6.86	108.54	105.80
1	AA	608	A	C5-N7-C8	6.86	107.33	103.90
1	AA	694	A	C4-C5-C6	6.86	120.43	117.00
22	BA	182	A	N9-C4-C5	6.86	108.54	105.80
22	BA	666	A	C5-N7-C8	6.86	107.33	103.90
22	BA	793	A	C5-N7-C8	6.86	107.33	103.90
22	BA	1103	A	N9-C4-C5	6.86	108.54	105.80
1	AA	66	A	C4-C5-C6	6.86	120.43	117.00
1	AA	729	A	C4-C5-C6	6.86	120.43	117.00
1	AA	1513	A	C4-C5-C6	6.86	120.43	117.00
22	BA	928	A	C4-C5-C6	6.85	120.43	117.00
22	BA	943	A	N9-C4-C5	6.85	108.54	105.80
22	BA	2705	A	C5-N7-C8	6.85	107.33	103.90
1	AA	702	A	N9-C4-C5	6.85	108.54	105.80
1	AA	802	A	C5-N7-C8	6.85	107.33	103.90
22	BA	602	A	N9-C4-C5	6.85	108.54	105.80
22	BA	2225	A	C5-N7-C8	6.85	107.33	103.90
1	AA	50	A	C4-C5-C6	6.85	120.42	117.00
1	AA	1254	A	C4-C5-C6	6.85	120.42	117.00
22	BA	84	A	C5-N7-C8	6.85	107.32	103.90
22	BA	1328	A	N9-C4-C5	6.85	108.54	105.80
22	BA	1901	A	N9-C4-C5	6.85	108.54	105.80
23	BB	39	A	C5-N7-C8	6.85	107.32	103.90
1	AA	520	A	C4-C5-N7	-6.85	107.28	110.70
1	AA	182	A	C5-N7-C8	6.84	107.32	103.90
22	BA	231	A	C4-C5-N7	-6.84	107.28	110.70
22	BA	928	A	N9-C4-C5	6.84	108.54	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1791	A	C5-N7-C8	6.84	107.32	103.90
22	BA	2126	A	C5-N7-C8	6.84	107.32	103.90
22	BA	2518	A	N3-C4-N9	6.84	132.88	127.40
22	BA	2781	A	C5-N7-C8	6.84	107.32	103.90
23	BB	45	A	N9-C4-C5	6.84	108.54	105.80
1	AA	32	A	N3-C4-N9	6.84	132.88	127.40
22	BA	2682	A	N9-C4-C5	6.84	108.54	105.80
1	AA	7	A	N9-C4-C5	6.84	108.54	105.80
1	AA	98	A	N9-C4-C5	6.84	108.54	105.80
22	BA	1900	A	C4-C5-C6	6.84	120.42	117.00
1	AA	182	A	N9-C4-C5	6.84	108.54	105.80
1	AA	983	A	N9-C4-C5	6.84	108.54	105.80
22	BA	256	A	C5-N7-C8	6.84	107.32	103.90
22	BA	505	A	C5-N7-C8	6.84	107.32	103.90
22	BA	1496	A	C5-N7-C8	6.84	107.32	103.90
1	AA	1299	A	N3-C4-N9	6.84	132.87	127.40
22	BA	320	A	C5-N7-C8	6.84	107.32	103.90
22	BA	802	A	N3-C4-N9	6.84	132.87	127.40
1	AA	607	A	C4-C5-C6	6.84	120.42	117.00
22	BA	984	A	C4-C5-C6	6.84	120.42	117.00
22	BA	2267	A	C5-N7-C8	6.84	107.32	103.90
1	AA	466	A	C4-C5-C6	6.83	120.42	117.00
1	AA	1204	A	C4-C5-N7	-6.83	107.28	110.70
1	AA	1261	A	C4-C5-C6	6.83	120.42	117.00
22	BA	794	A	C4-C5-C6	6.83	120.42	117.00
22	BA	2037	A	C5-N7-C8	6.83	107.32	103.90
1	AA	452	A	C4-C5-C6	6.83	120.42	117.00
22	BA	1916	A	C5-N7-C8	6.83	107.32	103.90
22	BA	439	A	N9-C4-C5	6.83	108.53	105.80
1	AA	344	A	N9-C4-C5	6.83	108.53	105.80
1	AA	1350	A	N9-C4-C5	6.83	108.53	105.80
22	BA	103	A	N9-C4-C5	6.83	108.53	105.80
22	BA	782	A	C5-N7-C8	6.83	107.31	103.90
22	BA	2662	A	C5-N7-C8	6.83	107.31	103.90
1	AA	1257	A	N9-C4-C5	6.83	108.53	105.80
22	BA	1308	A	C4-C5-C6	6.82	120.41	117.00
22	BA	1503	A	N9-C4-C5	6.82	108.53	105.80
22	BA	216	A	C4-C5-C6	6.82	120.41	117.00
22	BA	1213	A	N3-C4-N9	6.82	132.86	127.40
23	BB	59	A	C5-C6-N6	6.82	129.16	123.70
55	B8	51	A	C8-N9-C4	6.82	108.53	105.80
1	AA	1508	A	C5-N7-C8	6.82	107.31	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	977	A	C4-C5-C6	6.82	120.41	117.00
22	BA	348	A	N9-C4-C5	6.82	108.53	105.80
22	BA	960	A	N3-C4-N9	6.82	132.85	127.40
22	BA	1871	A	N9-C4-C5	6.82	108.53	105.80
22	BA	2080	A	C4-C5-C6	6.82	120.41	117.00
1	AA	431	A	C4-C5-N7	-6.82	107.29	110.70
22	BA	156	A	C4-C5-C6	6.82	120.41	117.00
22	BA	1705	A	C4-C5-C6	6.82	120.41	117.00
22	BA	2135	A	C5-N7-C8	6.82	107.31	103.90
22	BA	345	A	C5-N7-C8	6.81	107.31	103.90
22	BA	574	A	C5-N7-C8	6.81	107.31	103.90
22	BA	1876	A	C4-C5-C6	6.81	120.41	117.00
1	AA	1324	A	C5-N7-C8	6.81	107.31	103.90
22	BA	693	A	C4-C5-C6	6.81	120.41	117.00
1	AA	460	A	C5-C6-N1	6.81	121.11	117.70
1	AA	149	A	C4-C5-C6	6.81	120.40	117.00
22	BA	943	A	C4-C5-C6	6.81	120.41	117.00
22	BA	1626	A	C5-N7-C8	6.81	107.31	103.90
22	BA	2435	A	C5-N7-C8	6.81	107.30	103.90
54	B7	9	A	N9-C4-C5	6.81	108.52	105.80
1	AA	435	A	N9-C4-C5	6.81	108.52	105.80
1	AA	1318	A	N9-C4-C5	6.81	108.52	105.80
22	BA	457	A	C4-C5-N7	-6.81	107.30	110.70
1	AA	546	A	C4-C5-C6	6.80	120.40	117.00
22	BA	722	A	C4-C5-C6	6.80	120.40	117.00
22	BA	2560	A	N9-C4-C5	6.80	108.52	105.80
22	BA	2679	A	N3-C4-N9	6.80	132.84	127.40
22	BA	222	A	N9-C4-C5	6.80	108.52	105.80
22	BA	2547	A	N9-C4-C5	6.80	108.52	105.80
22	BA	2740	A	C4-C5-C6	6.80	120.40	117.00
22	BA	272	A	C5-N7-C8	6.80	107.30	103.90
22	BA	722	A	C5-N7-C8	6.80	107.30	103.90
22	BA	756	A	C4-C5-C6	6.80	120.40	117.00
22	BA	2873	A	N9-C4-C5	6.80	108.52	105.80
1	AA	1111	A	N9-C4-C5	6.80	108.52	105.80
1	AA	1534	A	C5-N7-C8	6.80	107.30	103.90
22	BA	63	A	C4-C5-C6	6.80	120.40	117.00
22	BA	996	A	C5-N7-C8	6.80	107.30	103.90
22	BA	2071	A	C5-N7-C8	6.80	107.30	103.90
22	BA	2328	A	C4-C5-C6	6.80	120.40	117.00
1	AA	300	A	N3-C4-N9	6.79	132.84	127.40
22	BA	176	A	C4-C5-C6	6.79	120.40	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2823	A	N9-C4-C5	6.79	108.52	105.80
1	AA	892	A	C5-N7-C8	6.79	107.30	103.90
22	BA	833	A	C5-N7-C8	6.79	107.30	103.90
1	AA	60	A	C4-C5-C6	6.79	120.40	117.00
1	AA	172	A	N9-C4-C5	6.79	108.52	105.80
22	BA	172	A	N9-C4-C5	6.79	108.52	105.80
22	BA	563	A	C4-C5-N7	-6.79	107.31	110.70
1	AA	535	A	N9-C4-C5	6.79	108.52	105.80
22	BA	2378	A	C4-C5-C6	6.79	120.39	117.00
1	AA	80	A	C4-C5-C6	6.79	120.39	117.00
1	AA	162	A	N3-C4-N9	6.79	132.83	127.40
22	BA	945	A	N9-C4-C5	6.79	108.51	105.80
22	BA	1413	A	C5-N7-C8	6.79	107.29	103.90
1	AA	120	A	N9-C4-C5	6.78	108.51	105.80
1	AA	415	A	N9-C4-C5	6.78	108.51	105.80
1	AA	648	A	C5-N7-C8	6.78	107.29	103.90
1	AA	649	A	N9-C4-C5	6.78	108.51	105.80
1	AA	687	A	C5-N7-C8	6.78	107.29	103.90
1	AA	777	A	N9-C4-C5	6.78	108.51	105.80
1	AA	872	A	N9-C4-C5	6.78	108.51	105.80
1	AA	1531	A	C5-N7-C8	6.78	107.29	103.90
22	BA	1652	A	C5-N7-C8	6.78	107.29	103.90
1	AA	629	A	C5-N7-C8	6.78	107.29	103.90
1	AA	1036	A	N9-C4-C5	6.78	108.51	105.80
1	AA	1236	A	N9-C4-C5	6.78	108.51	105.80
1	AA	1239	A	C5-N7-C8	6.78	107.29	103.90
1	AA	1252	A	C5-N7-C8	6.78	107.29	103.90
1	AA	1280	A	N9-C4-C5	6.78	108.51	105.80
22	BA	1321	A	C4-C5-C6	6.78	120.39	117.00
1	AA	270	A	C5-N7-C8	6.78	107.29	103.90
1	AA	1236	A	C5-N7-C8	6.78	107.29	103.90
1	AA	461	A	C5-N7-C8	6.78	107.29	103.90
1	AA	1093	A	C4-C5-C6	6.78	120.39	117.00
22	BA	980	A	N3-C4-N9	6.78	132.82	127.40
22	BA	2135	A	C4-C5-C6	6.78	120.39	117.00
22	BA	2589	A	N9-C4-C5	6.78	108.51	105.80
23	BB	29	A	N9-C4-C5	6.78	108.51	105.80
23	BB	66	A	C4-C5-C6	6.78	120.39	117.00
1	AA	432	A	C4-C5-C6	6.77	120.39	117.00
22	BA	13	A	C4-C5-C6	6.77	120.39	117.00
22	BA	1608	A	C4-C5-C6	6.77	120.39	117.00
1	AA	1150	A	N9-C4-C5	6.77	108.51	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2381	A	N9-C4-C5	6.77	108.51	105.80
22	BA	2761	A	C4-C5-C6	6.77	120.39	117.00
22	BA	1028	A	C5-N7-C8	6.77	107.29	103.90
22	BA	2134	A	N9-C4-C5	6.77	108.51	105.80
22	BA	2657	A	C5-N7-C8	6.77	107.28	103.90
1	AA	356	A	N9-C4-C5	6.77	108.51	105.80
22	BA	2268	A	N9-C4-C5	6.77	108.51	105.80
22	BA	482	A	N3-C4-N9	6.76	132.81	127.40
1	AA	189	A	N9-C4-C5	6.76	108.50	105.80
1	AA	338	A	N9-C4-C5	6.76	108.50	105.80
1	AA	937	A	C4-C5-C6	6.76	120.38	117.00
22	BA	1900	A	N9-C4-C5	6.76	108.50	105.80
22	BA	626	A	C4-C5-C6	6.76	120.38	117.00
22	BA	2814	A	N9-C4-C5	6.76	108.50	105.80
1	AA	74	A	C4-C5-N7	-6.76	107.32	110.70
22	BA	706	A	N9-C4-C5	6.76	108.50	105.80
22	BA	1802	A	N9-C4-C5	6.76	108.50	105.80
1	AA	172	A	C5-N7-C8	6.76	107.28	103.90
1	AA	456	A	N9-C4-C5	6.76	108.50	105.80
22	BA	251	A	N3-C4-N9	6.76	132.81	127.40
22	BA	1746	A	C5-N7-C8	6.76	107.28	103.90
22	BA	2476	A	C5-N7-C8	6.76	107.28	103.90
1	AA	33	A	C4-C5-C6	6.75	120.38	117.00
1	AA	493	A	C5-N7-C8	6.75	107.28	103.90
22	BA	877	A	C5-N7-C8	6.75	107.28	103.90
22	BA	1354	A	C4-C5-C6	6.75	120.38	117.00
23	BB	50	A	C5-N7-C8	6.75	107.28	103.90
1	AA	978	A	C4-C5-C6	6.75	120.38	117.00
1	AA	1082	A	C5-N7-C8	6.75	107.28	103.90
22	BA	1981	A	N9-C4-C5	6.75	108.50	105.80
22	BA	2191	A	C5-N7-C8	6.75	107.28	103.90
22	BA	2883	A	N9-C4-C5	6.75	108.50	105.80
1	AA	539	A	C5-N7-C8	6.75	107.28	103.90
1	AA	975	A	N9-C4-C5	6.75	108.50	105.80
22	BA	1650	A	N3-C4-N9	6.75	132.80	127.40
1	AA	718	A	C5-N7-C8	6.75	107.27	103.90
1	AA	1288	A	N9-C4-C5	6.75	108.50	105.80
22	BA	2317	A	C4-C5-C6	6.75	120.37	117.00
1	AA	1130	A	C4-C5-C6	6.74	120.37	117.00
1	AA	1225	A	N9-C4-C5	6.74	108.50	105.80
22	BA	750	A	N3-C4-N9	6.74	132.79	127.40
22	BA	1347	A	N9-C4-C5	6.74	108.50	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1809	A	C5-N7-C8	6.74	107.27	103.90
22	BA	1901	A	C5-N7-C8	6.74	107.27	103.90
22	BA	2015	A	C5-N7-C8	6.74	107.27	103.90
1	AA	649	A	C4-C5-C6	6.74	120.37	117.00
1	AA	815	A	C5-N7-C8	6.74	107.27	103.90
2	AB	188	ASP	OD1-CG-OD2	-6.74	110.49	123.30
22	BA	256	A	C4-C5-C6	6.74	120.37	117.00
22	BA	632	A	C4-C5-C6	6.74	120.37	117.00
22	BA	756	A	C5-N7-C8	6.74	107.27	103.90
22	BA	2439	A	C5-N7-C8	6.74	107.27	103.90
1	AA	831	A	N9-C4-C5	6.74	108.50	105.80
1	AA	1446	A	C5-N7-C8	6.74	107.27	103.90
22	BA	310	A	C5-N7-C8	6.74	107.27	103.90
22	BA	621	A	C5-N7-C8	6.74	107.27	103.90
22	BA	849	A	C5-N7-C8	6.74	107.27	103.90
22	BA	1419	A	C5-N7-C8	6.74	107.27	103.90
1	AA	1081	A	C4-C5-C6	6.73	120.37	117.00
22	BA	131	A	N3-C4-N9	6.73	132.79	127.40
22	BA	310	A	N9-C4-C5	6.73	108.49	105.80
22	BA	348	A	C4-C5-C6	6.73	120.37	117.00
22	BA	1205	A	C4-C5-C6	6.73	120.36	117.00
22	BA	1285	A	C4-C5-C6	6.73	120.36	117.00
22	BA	1509	A	N9-C4-C5	6.73	108.49	105.80
22	BA	1603	A	C4-C5-C6	6.73	120.36	117.00
22	BA	2013	A	C4-C5-C6	6.73	120.36	117.00
22	BA	391	A	C5-N7-C8	6.73	107.27	103.90
22	BA	1928	A	N9-C4-C5	6.73	108.49	105.80
55	B8	38	A	C5-N7-C8	6.73	107.27	103.90
1	AA	655	A	N9-C4-C5	6.73	108.49	105.80
22	BA	2176	A	C4-C5-C6	6.73	120.36	117.00
1	AA	116	A	C5-N7-C8	6.72	107.26	103.90
1	AA	559	A	C5-N7-C8	6.72	107.26	103.90
1	AA	1236	A	C4-C5-C6	6.72	120.36	117.00
1	AA	1433	A	C5-N7-C8	6.72	107.26	103.90
22	BA	218	A	N9-C4-C5	6.72	108.49	105.80
22	BA	1189	A	N3-C4-N9	6.72	132.78	127.40
22	BA	2227	A	C4-C5-C6	6.72	120.36	117.00
22	BA	233	A	C4-C5-C6	6.72	120.36	117.00
22	BA	1272	A	N9-C4-C5	6.72	108.49	105.80
22	BA	721	A	C4-C5-C6	6.72	120.36	117.00
22	BA	1274	A	C4-C5-C6	6.72	120.36	117.00
23	BB	34	A	C5-N7-C8	6.72	107.26	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	251	A	C5-N7-C8	6.72	107.26	103.90
22	BA	497	A	N9-C4-C5	6.72	108.49	105.80
22	BA	508	A	N9-C4-C5	6.72	108.49	105.80
22	BA	1689	A	C4-C5-C6	6.72	120.36	117.00
22	BA	1854	A	C5-N7-C8	6.72	107.26	103.90
22	BA	2766	A	N3-C4-N9	6.72	132.78	127.40
55	B8	66	A	C5-N7-C8	6.72	107.26	103.90
1	AA	1319	A	C5-N7-C8	6.72	107.26	103.90
22	BA	74	A	N9-C4-C5	6.72	108.49	105.80
22	BA	1591	A	C5-N7-C8	6.72	107.26	103.90
22	BA	2199	A	C5-N7-C8	6.72	107.26	103.90
1	AA	782	A	C4-C5-C6	6.71	120.36	117.00
22	BA	53	A	C5-N7-C8	6.71	107.26	103.90
22	BA	492	A	N9-C4-C5	6.71	108.49	105.80
1	AA	1408	A	N9-C4-C5	6.71	108.48	105.80
1	AA	77	A	C5-N7-C8	6.71	107.26	103.90
1	AA	192	A	C4-C5-C6	6.71	120.36	117.00
1	AA	441	A	N9-C4-C5	6.71	108.48	105.80
1	AA	729	A	C5-N7-C8	6.71	107.26	103.90
22	BA	844	A	C5-N7-C8	6.71	107.26	103.90
22	BA	2327	A	C4-C5-C6	6.71	120.36	117.00
22	BA	181	A	C4-C5-C6	6.71	120.36	117.00
22	BA	1126	A	C5-N7-C8	6.71	107.25	103.90
1	AA	71	A	C5-N7-C8	6.71	107.25	103.90
1	AA	389	A	C5-N7-C8	6.71	107.25	103.90
1	AA	1239	A	C8-N9-C4	6.71	108.48	105.80
22	BA	279	A	N9-C4-C5	6.71	108.48	105.80
22	BA	1717	A	C4-C5-C6	6.71	120.36	117.00
1	AA	50	A	C5-N7-C8	6.71	107.25	103.90
22	BA	1713	A	C5-N7-C8	6.71	107.25	103.90
22	BA	324	A	C4-C5-C6	6.71	120.35	117.00
22	BA	300	A	C5-N7-C8	6.70	107.25	103.90
22	BA	1494	A	C5-N7-C8	6.70	107.25	103.90
22	BA	1641	A	N9-C4-C5	6.70	108.48	105.80
22	BA	2660	A	N9-C4-C5	6.70	108.48	105.80
1	AA	228	A	C5-N7-C8	6.70	107.25	103.90
22	BA	226	A	C4-C5-C6	6.70	120.35	117.00
22	BA	332	A	N9-C4-C5	6.70	108.48	105.80
1	AA	1157	A	C4-C5-C6	6.70	120.35	117.00
22	BA	1572	A	N9-C4-C5	6.70	108.48	105.80
22	BA	1885	A	C5-N7-C8	6.70	107.25	103.90
22	BA	2126	A	C4-C5-C6	6.70	120.35	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	451	A	N9-C4-C5	6.70	108.48	105.80
22	BA	1327	A	C4-C5-C6	6.70	120.35	117.00
22	BA	2097	A	C5-N7-C8	6.70	107.25	103.90
1	AA	1080	A	N9-C4-C5	6.70	108.48	105.80
1	AA	10	A	C4-C5-C6	6.70	120.35	117.00
22	BA	1603	A	N3-C4-N9	6.70	132.76	127.40
22	BA	1650	A	C4-C5-C6	6.70	120.35	117.00
1	AA	1349	A	N9-C4-C5	6.69	108.48	105.80
1	AA	1508	A	N9-C4-C5	6.69	108.48	105.80
22	BA	191	A	C4-C5-N7	-6.69	107.35	110.70
22	BA	2654	A	C5-N7-C8	6.69	107.25	103.90
22	BA	2721	A	N9-C4-C5	6.69	108.48	105.80
1	AA	1396	A	C5-N7-C8	6.69	107.25	103.90
22	BA	996	A	C4-C5-C6	6.69	120.35	117.00
22	BA	1745	A	C5-N7-C8	6.69	107.25	103.90
22	BA	2516	A	C4-C5-C6	6.69	120.35	117.00
1	AA	288	A	C5-N7-C8	6.69	107.25	103.90
22	BA	223	A	C5-N7-C8	6.69	107.25	103.90
23	BB	108	A	C5-N7-C8	6.69	107.25	103.90
1	AA	279	A	N9-C4-C5	6.69	108.48	105.80
22	BA	432	A	N9-C4-C5	6.69	108.47	105.80
22	BA	1932	A	C5-N7-C8	6.69	107.25	103.90
1	AA	602	A	C4-C5-C6	6.69	120.34	117.00
1	AA	1362	A	N9-C4-C5	6.69	108.47	105.80
22	BA	1650	A	N9-C4-C5	6.69	108.47	105.80
1	AA	499	A	N9-C4-C5	6.69	108.47	105.80
23	BB	94	A	C5-N7-C8	6.69	107.24	103.90
1	AA	702	A	C4-C5-C6	6.68	120.34	117.00
1	AA	1213	A	C4-C5-N7	-6.68	107.36	110.70
22	BA	918	A	N9-C4-C5	6.68	108.47	105.80
23	BB	73	A	C4-C5-C6	6.68	120.34	117.00
1	AA	523	A	C5-N7-C8	6.68	107.24	103.90
22	BA	1040	A	N9-C4-C5	6.68	108.47	105.80
22	BA	1900	A	C5-N7-C8	6.68	107.24	103.90
22	BA	2450	A	C4-C5-C6	6.68	120.34	117.00
22	BA	861	A	C5-N7-C8	6.68	107.24	103.90
22	BA	2114	A	C5-N7-C8	6.68	107.24	103.90
1	AA	374	A	C4-C5-C6	6.68	120.34	117.00
1	AA	629	A	N9-C4-C5	6.68	108.47	105.80
1	AA	704	A	C5-N7-C8	6.68	107.24	103.90
22	BA	1634	A	C5-N7-C8	6.68	107.24	103.90
1	AA	174	A	N9-C4-C5	6.68	108.47	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	16	A	C4-C5-C6	6.68	120.34	117.00
1	AA	1188	A	C4-C5-C6	6.68	120.34	117.00
22	BA	19	A	C4-C5-C6	6.68	120.34	117.00
22	BA	430	A	C5-N7-C8	6.68	107.24	103.90
22	BA	1419	A	N9-C4-C5	6.68	108.47	105.80
22	BA	1801	A	C4-C5-C6	6.68	120.34	117.00
1	AA	1280	A	C5-N7-C8	6.67	107.24	103.90
1	AA	1456	A	C4-C5-C6	6.67	120.34	117.00
22	BA	1522	A	N9-C4-C5	6.67	108.47	105.80
22	BA	1591	A	C4-C5-C6	6.67	120.34	117.00
22	BA	1858	A	N9-C4-C5	6.67	108.47	105.80
22	BA	2142	A	N3-C4-N9	6.67	132.74	127.40
1	AA	71	A	N9-C4-C5	6.67	108.47	105.80
1	AA	468	A	N9-C4-C5	6.67	108.47	105.80
22	BA	920	A	C4-C5-C6	6.67	120.33	117.00
22	BA	2733	A	C4-C5-C6	6.67	120.33	117.00
1	AA	635	A	N9-C4-C5	6.67	108.47	105.80
22	BA	749	A	C4-C5-C6	6.67	120.33	117.00
23	BB	108	A	N9-C4-C5	6.67	108.47	105.80
1	AA	780	A	N9-C4-C5	6.66	108.47	105.80
22	BA	1819	A	C4-C5-N7	-6.66	107.37	110.70
1	AA	468	A	C4-C5-C6	6.66	120.33	117.00
22	BA	172	A	C4-C5-C6	6.66	120.33	117.00
1	AA	1163	A	N3-C4-N9	6.66	132.73	127.40
22	BA	2406	A	N9-C4-C5	6.66	108.46	105.80
22	BA	2893	A	C5-N7-C8	6.66	107.23	103.90
1	AA	1180	A	C4-C5-C6	6.66	120.33	117.00
22	BA	453	A	C4-C5-C6	6.66	120.33	117.00
22	BA	676	A	C5-N7-C8	6.66	107.23	103.90
1	AA	609	A	C4-C5-C6	6.66	120.33	117.00
22	BA	402	A	N9-C4-C5	6.66	108.46	105.80
22	BA	2386	A	C4-C5-C6	6.66	120.33	117.00
1	AA	1339	A	C5-N7-C8	6.65	107.23	103.90
1	AA	1105	A	N9-C4-C5	6.65	108.46	105.80
22	BA	632	A	C5-N7-C8	6.65	107.23	103.90
22	BA	1477	A	C5-N7-C8	6.65	107.23	103.90
22	BA	2358	A	C4-C5-C6	6.65	120.33	117.00
22	BA	2765	A	N3-C4-N9	6.65	132.72	127.40
1	AA	663	A	C5-N7-C8	6.65	107.22	103.90
22	BA	505	A	N9-C4-C5	6.65	108.46	105.80
22	BA	1505	A	N9-C4-C5	6.65	108.46	105.80
22	BA	1805	A	C4-C5-C6	6.65	120.33	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	865	A	C5-N7-C8	6.65	107.22	103.90
22	BA	1014	A	C4-C5-C6	6.65	120.32	117.00
22	BA	1495	A	C5-N7-C8	6.65	107.22	103.90
22	BA	2333	A	C5-N7-C8	6.65	107.22	103.90
22	BA	1786	A	N9-C4-C5	6.65	108.46	105.80
1	AA	532	A	C5-N7-C8	6.64	107.22	103.90
1	AA	695	A	N9-C4-C5	6.64	108.46	105.80
22	BA	1133	A	N9-C4-C5	6.64	108.46	105.80
22	BA	1803	A	N9-C4-C5	6.64	108.46	105.80
22	BA	2267	A	C4-C5-C6	6.64	120.32	117.00
22	BA	2534	A	N9-C4-C5	6.64	108.46	105.80
1	AA	460	A	N9-C4-C5	6.64	108.46	105.80
22	BA	101	A	C5-N7-C8	6.64	107.22	103.90
22	BA	522	A	N9-C4-C5	6.64	108.46	105.80
1	AA	1005	A	N9-C4-C5	6.64	108.46	105.80
1	AA	1042	A	N9-C4-C5	6.64	108.46	105.80
22	BA	156	A	C5-N7-C8	6.64	107.22	103.90
22	BA	689	A	C4-C5-C6	6.64	120.32	117.00
22	BA	988	A	N9-C4-C5	6.64	108.46	105.80
1	AA	321	A	N9-C4-C5	6.64	108.46	105.80
1	AA	583	A	C4-C5-C6	6.64	120.32	117.00
1	AA	602	A	N9-C4-C5	6.64	108.45	105.80
22	BA	63	A	C5-N7-C8	6.64	107.22	103.90
22	BA	2565	A	C5-N7-C8	6.64	107.22	103.90
23	BB	58	A	N9-C4-C5	6.64	108.45	105.80
54	B7	9	A	C5-N7-C8	6.64	107.22	103.90
1	AA	1000	A	C4-C5-C6	6.64	120.32	117.00
22	BA	1598	A	N9-C4-C5	6.64	108.45	105.80
1	AA	1225	A	C4-C5-C6	6.64	120.32	117.00
22	BA	1608	A	C5-N7-C8	6.63	107.22	103.90
22	BA	1616	A	N9-C4-C5	6.63	108.45	105.80
22	BA	2432	A	C5-N7-C8	6.63	107.22	103.90
22	BA	781	A	C4-C5-C6	6.63	120.32	117.00
1	AA	298	A	C4-C5-C6	6.63	120.31	117.00
1	AA	937	A	N9-C4-C5	6.63	108.45	105.80
1	AA	1157	A	N9-C4-C5	6.63	108.45	105.80
22	BA	670	A	C5-N7-C8	6.63	107.22	103.90
22	BA	1403	A	C4-C5-C6	6.63	120.32	117.00
1	AA	382	A	N9-C4-C5	6.63	108.45	105.80
22	BA	155	A	C5-N7-C8	6.63	107.22	103.90
22	BA	345	A	C4-C5-C6	6.63	120.31	117.00
22	BA	1916	A	N9-C4-C5	6.63	108.45	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	59	A	N9-C4-C5	6.63	108.45	105.80
1	AA	1430	A	C5-N7-C8	6.63	107.21	103.90
22	BA	794	A	C5-C6-N1	6.63	121.01	117.70
22	BA	2247	A	N9-C4-C5	6.63	108.45	105.80
1	AA	1507	A	N9-C4-C5	6.62	108.45	105.80
22	BA	1580	A	N9-C4-C5	6.62	108.45	105.80
1	AA	1349	A	C5-N7-C8	6.62	107.21	103.90
22	BA	504	A	C8-N9-C4	6.62	108.45	105.80
22	BA	972	A	C5-N7-C8	6.62	107.21	103.90
1	AA	553	A	C4-C5-C6	6.62	120.31	117.00
1	AA	716	A	C4-C5-C6	6.62	120.31	117.00
1	AA	1531	A	N9-C4-C5	6.62	108.45	105.80
1	AA	1036	A	C4-C5-C6	6.62	120.31	117.00
1	AA	1117	A	N9-C4-C5	6.62	108.45	105.80
22	BA	1067	A	N9-C4-C5	6.62	108.45	105.80
22	BA	1226	A	C5-N7-C8	6.62	107.21	103.90
22	BA	2734	A	N9-C4-C5	6.62	108.45	105.80
22	BA	2886	A	C4-C5-C6	6.62	120.31	117.00
22	BA	676	A	C4-C5-C6	6.62	120.31	117.00
22	BA	1275	A	N9-C4-C5	6.62	108.45	105.80
22	BA	1890	A	C4-C5-C6	6.61	120.31	117.00
22	BA	2823	A	C4-C5-C6	6.61	120.31	117.00
22	BA	743	A	C4-C5-C6	6.61	120.31	117.00
55	B8	76	A	C8-N9-C4	6.61	108.44	105.80
1	AA	199	A	N9-C4-C5	6.61	108.44	105.80
1	AA	1248	A	C4-C5-C6	6.61	120.30	117.00
22	BA	1086	A	N9-C4-C5	6.61	108.44	105.80
22	BA	1528	A	N3-C4-N9	6.61	132.69	127.40
1	AA	26	A	N9-C4-C5	6.61	108.44	105.80
1	AA	262	A	N9-C4-C5	6.61	108.44	105.80
1	AA	747	A	N9-C4-C5	6.61	108.44	105.80
22	BA	1535	A	C5-N7-C8	6.61	107.20	103.90
22	BA	2336	A	C5-N7-C8	6.61	107.20	103.90
1	AA	687	A	C4-C5-C6	6.61	120.30	117.00
1	AA	728	A	C4-C5-C6	6.61	120.30	117.00
1	AA	1507	A	C5-N7-C8	6.61	107.20	103.90
22	BA	362	A	C5-N7-C8	6.61	107.20	103.90
22	BA	6	A	C4-C5-C6	6.60	120.30	117.00
22	BA	1912	A	N9-C4-C5	6.60	108.44	105.80
1	AA	81	A	C4-C5-C6	6.60	120.30	117.00
1	AA	574	A	C5-N7-C8	6.60	107.20	103.90
1	AA	1275	A	C4-C5-C6	6.60	120.30	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	429	A	N9-C4-C5	6.60	108.44	105.80
22	BA	927	A	N9-C4-C5	6.60	108.44	105.80
22	BA	1805	A	N9-C4-C5	6.60	108.44	105.80
1	AA	1288	A	C5-N7-C8	6.60	107.20	103.90
22	BA	1596	A	N9-C4-C5	6.60	108.44	105.80
1	AA	10	A	N9-C4-C5	6.60	108.44	105.80
1	AA	630	A	C4-C5-C6	6.60	120.30	117.00
22	BA	1090	A	N9-C4-C5	6.60	108.44	105.80
22	BA	1387	A	C5-N7-C8	6.60	107.20	103.90
22	BA	2015	A	C4-C5-C6	6.60	120.30	117.00
22	BA	2893	A	C4-C5-C6	6.60	120.30	117.00
1	AA	143	A	C4-C5-C6	6.60	120.30	117.00
22	BA	1246	A	C4-C5-N7	-6.60	107.40	110.70
22	BA	2088	A	C5-N7-C8	6.60	107.20	103.90
22	BA	447	A	C4-C5-C6	6.60	120.30	117.00
22	BA	944	C	C5-C4-N4	6.60	124.82	120.20
55	B8	41	A	C8-N9-C4	6.60	108.44	105.80
1	AA	161	A	N9-C4-C5	6.59	108.44	105.80
22	BA	14	A	C5-N7-C8	6.59	107.20	103.90
22	BA	1308	A	C4-C5-N7	-6.59	107.40	110.70
22	BA	1783	A	C5-N7-C8	6.59	107.20	103.90
22	BA	1877	A	C4-C5-C6	6.59	120.30	117.00
1	AA	1	A	C5-N7-C8	6.59	107.20	103.90
1	AA	306	A	N9-C4-C5	6.59	108.44	105.80
1	AA	1176	A	C5-N7-C8	6.59	107.20	103.90
22	BA	197	A	C5-N7-C8	6.59	107.20	103.90
22	BA	272	A	C4-C5-C6	6.59	120.30	117.00
1	AA	914	A	C4-C5-C6	6.59	120.30	117.00
22	BA	1367	A	C4-C5-C6	6.59	120.30	117.00
22	BA	1690	A	C5-N7-C8	6.59	107.19	103.90
22	BA	1746	A	C4-C5-C6	6.59	120.30	117.00
1	AA	478	A	C4-C5-C6	6.59	120.30	117.00
22	BA	49	A	C4-C5-C6	6.59	120.30	117.00
22	BA	1366	A	C4-C5-C6	6.59	120.30	117.00
22	BA	1586	A	C4-C5-C6	6.59	120.29	117.00
22	BA	2005	A	N9-C4-C5	6.59	108.44	105.80
22	BA	532	A	N9-C4-C5	6.59	108.44	105.80
22	BA	1640	A	C5-C6-N1	6.59	120.99	117.70
22	BA	181	A	N9-C4-C5	6.59	108.43	105.80
1	AA	909	A	C5-N7-C8	6.58	107.19	103.90
1	AA	994	A	N9-C4-C5	6.58	108.43	105.80
1	AA	80	A	N9-C4-C5	6.58	108.43	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	250	A	C5-N7-C8	6.58	107.19	103.90
1	AA	864	A	C5-N7-C8	6.58	107.19	103.90
1	AA	1318	A	C5-N7-C8	6.58	107.19	103.90
1	AA	635	A	C4-C5-C6	6.58	120.29	117.00
1	AA	938	A	N3-C4-N9	6.58	132.66	127.40
1	AA	759	A	N9-C4-C5	6.58	108.43	105.80
22	BA	844	A	C4-C5-C6	6.58	120.29	117.00
22	BA	1265	A	C4-C5-C6	6.58	120.29	117.00
1	AA	968	A	N9-C4-C5	6.58	108.43	105.80
22	BA	878	A	N9-C4-C5	6.58	108.43	105.80
22	BA	2278	A	C4-C5-C6	6.58	120.29	117.00
22	BA	1342	A	N9-C4-C5	6.58	108.43	105.80
22	BA	1579	A	C4-C5-C6	6.58	120.29	117.00
1	AA	608	A	C4-C5-C6	6.57	120.29	117.00
1	AA	1285	A	N9-C4-C5	6.57	108.43	105.80
22	BA	1070	A	N9-C4-C5	6.57	108.43	105.80
22	BA	1953	A	N9-C4-C5	6.57	108.43	105.80
22	BA	2169	A	C4-C5-C6	6.57	120.29	117.00
1	AA	1502	A	N9-C4-C5	6.57	108.43	105.80
22	BA	510	C	C6-N1-C2	-6.57	117.67	120.30
22	BA	1328	A	C4-C5-C6	6.57	120.28	117.00
22	BA	2868	A	C4-C5-C6	6.57	120.28	117.00
1	AA	600	A	N9-C4-C5	6.57	108.43	105.80
1	AA	1082	A	C4-C5-C6	6.57	120.28	117.00
1	AA	389	A	N9-C4-C5	6.57	108.43	105.80
22	BA	644	A	N9-C4-C5	6.57	108.43	105.80
22	BA	1640	A	C5-N7-C8	6.56	107.18	103.90
22	BA	2433	A	C4-C5-C6	6.56	120.28	117.00
1	AA	640	A	C4-C5-C6	6.56	120.28	117.00
1	AA	1534	A	C4-C5-C6	6.56	120.28	117.00
22	BA	89	A	N9-C4-C5	6.56	108.42	105.80
22	BA	1050	A	C4-C5-C6	6.56	120.28	117.00
1	AA	1274	A	C5-N7-C8	6.56	107.18	103.90
22	BA	819	A	N3-C4-N9	6.56	132.65	127.40
22	BA	1301	A	C4-C5-C6	6.56	120.28	117.00
1	AA	1216	A	C4-C5-C6	6.56	120.28	117.00
22	BA	1175	A	C5-N7-C8	6.56	107.18	103.90
22	BA	1433	A	C5-N7-C8	6.56	107.18	103.90
22	BA	1502	A	C4-C5-C6	6.56	120.28	117.00
22	BA	2117	A	N9-C4-C5	6.56	108.42	105.80
1	AA	397	A	C5-N7-C8	6.56	107.18	103.90
1	AA	759	A	C4-C5-C6	6.56	120.28	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1155	A	N9-C4-C5	6.56	108.42	105.80
22	BA	6	A	C5-N7-C8	6.56	107.18	103.90
22	BA	347	A	C4-C5-C6	6.56	120.28	117.00
22	BA	2059	A	N9-C4-C5	6.56	108.42	105.80
22	BA	1871	A	C4-C5-C6	6.56	120.28	117.00
1	AA	1067	A	N9-C4-C5	6.55	108.42	105.80
22	BA	1549	A	C4-C5-C6	6.55	120.28	117.00
22	BA	2778	A	N9-C4-C5	6.55	108.42	105.80
1	AA	600	A	C5-N7-C8	6.55	107.18	103.90
1	AA	1324	A	N9-C4-C5	6.55	108.42	105.80
22	BA	845	A	C5-N7-C8	6.55	107.18	103.90
1	AA	139	A	N9-C4-C5	6.55	108.42	105.80
1	AA	435	A	C4-C5-C6	6.55	120.28	117.00
22	BA	218	A	C5-N7-C8	6.55	107.18	103.90
22	BA	2660	A	C4-C5-C6	6.55	120.28	117.00
55	B8	59	A	N3-C4-N9	6.55	132.64	127.40
22	BA	730	A	N3-C4-N9	6.55	132.64	127.40
22	BA	2418	A	C4-C5-C6	6.55	120.28	117.00
23	BB	15	A	N9-C4-C5	6.55	108.42	105.80
55	B8	66	A	N3-C4-N9	6.55	132.64	127.40
1	AA	288	A	C4-C5-C6	6.55	120.27	117.00
1	AA	665	A	C5-N7-C8	6.55	107.17	103.90
1	AA	49	U	C5-C4-O4	6.55	129.83	125.90
1	AA	51	A	C4-C5-C6	6.55	120.27	117.00
1	AA	640	A	N9-C4-C5	6.55	108.42	105.80
1	AA	1219	A	C5-N7-C8	6.55	107.17	103.90
22	BA	1871	A	C5-N7-C8	6.55	107.17	103.90
22	BA	2108	A	N9-C4-C5	6.55	108.42	105.80
22	BA	2328	A	C5-N7-C8	6.54	107.17	103.90
1	AA	1110	A	C4-C5-C6	6.54	120.27	117.00
22	BA	1244	A	C4-C5-C6	6.54	120.27	117.00
22	BA	2476	A	C4-C5-C6	6.54	120.27	117.00
22	BA	2883	A	C4-C5-N7	-6.54	107.43	110.70
1	AA	681	A	C4-C5-C6	6.54	120.27	117.00
22	BA	1040	A	C4-C5-C6	6.54	120.27	117.00
22	BA	1676	A	C4-C5-C6	6.54	120.27	117.00
22	BA	715	A	C4-C5-C6	6.54	120.27	117.00
22	BA	28	A	C5-N7-C8	6.54	107.17	103.90
22	BA	56	A	C4-C5-C6	6.54	120.27	117.00
22	BA	244	A	C4-C5-C6	6.54	120.27	117.00
22	BA	616	A	C5-N7-C8	6.54	107.17	103.90
22	BA	739	A	N9-C4-C5	6.54	108.42	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1735	A	C4-C5-C6	6.54	120.27	117.00
1	AA	687	A	N9-C4-C5	6.54	108.41	105.80
1	AA	1169	A	C4-C5-C6	6.54	120.27	117.00
22	BA	1354	A	C5-N7-C8	6.54	107.17	103.90
22	BA	480	A	C5-N7-C8	6.53	107.17	103.90
22	BA	1669	A	C5-N7-C8	6.53	107.17	103.90
22	BA	483	A	N9-C4-C5	6.53	108.41	105.80
22	BA	2821	A	C4-C5-C6	6.53	120.27	117.00
22	BA	483	A	C4-C5-C6	6.53	120.27	117.00
55	B8	69	A	C8-N9-C4	6.53	108.41	105.80
22	BA	1008	A	N9-C4-C5	6.53	108.41	105.80
55	B8	59	A	C8-N9-C4	6.53	108.41	105.80
1	AA	532	A	C4-C5-C6	6.53	120.26	117.00
1	AA	935	A	C4-C5-C6	6.53	120.26	117.00
1	AA	949	A	C4-C5-C6	6.53	120.26	117.00
22	BA	990	A	C4-C5-C6	6.53	120.26	117.00
22	BA	2184	A	N9-C4-C5	6.53	108.41	105.80
22	BA	10	A	C5-N7-C8	6.53	107.16	103.90
22	BA	1133	A	C4-C5-C6	6.53	120.26	117.00
1	AA	298	A	N9-C4-C5	6.52	108.41	105.80
22	BA	900	A	N9-C4-C5	6.52	108.41	105.80
22	BA	2184	A	C4-C5-C6	6.52	120.26	117.00
22	BA	2297	A	N9-C4-C5	6.52	108.41	105.80
22	BA	477	A	C5-N7-C8	6.52	107.16	103.90
22	BA	1230	A	N9-C4-C5	6.52	108.41	105.80
22	BA	2765	A	C5-N7-C8	6.52	107.16	103.90
22	BA	28	A	N9-C4-C5	6.52	108.41	105.80
22	BA	1969	A	C4-C5-C6	6.52	120.26	117.00
22	BA	2288	A	N9-C4-C5	6.52	108.41	105.80
1	AA	130	A	N9-C4-C5	6.51	108.41	105.80
1	AA	253	A	C5-C6-N1	6.51	120.96	117.70
22	BA	1494	A	N9-C4-C5	6.51	108.41	105.80
22	BA	1593	A	N9-C4-C5	6.51	108.41	105.80
22	BA	1634	A	C4-C5-C6	6.51	120.26	117.00
22	BA	1918	A	N9-C4-C5	6.51	108.41	105.80
1	AA	1254	A	N9-C4-C5	6.51	108.41	105.80
1	AA	1274	A	C4-C5-C6	6.51	120.26	117.00
22	BA	983	A	C5-N7-C8	6.51	107.16	103.90
14	AN	46	LEU	CB-CG-CD1	-6.51	99.93	111.00
22	BA	1608	A	N9-C4-C5	6.51	108.40	105.80
22	BA	1609	A	C4-C5-C6	6.51	120.25	117.00
22	BA	167	A	N9-C4-C5	6.51	108.40	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	756	A	N9-C4-C5	6.51	108.40	105.80
22	BA	1284	A	C5-N7-C8	6.51	107.15	103.90
22	BA	1508	A	C4-C5-C6	6.50	120.25	117.00
22	BA	320	A	N9-C4-C5	6.50	108.40	105.80
22	BA	1085	A	N9-C4-C5	6.50	108.40	105.80
22	BA	1509	A	C4-C5-C6	6.50	120.25	117.00
1	AA	746	A	C5-N7-C8	6.50	107.15	103.90
1	AA	816	A	C4-C5-C6	6.50	120.25	117.00
22	BA	1928	A	C5-N7-C8	6.50	107.15	103.90
22	BA	2654	A	N9-C4-C5	6.50	108.40	105.80
22	BA	693	A	N3-C4-N9	6.50	132.60	127.40
22	BA	866	A	N9-C4-C5	6.50	108.40	105.80
22	BA	2095	A	C4-C5-N7	-6.50	107.45	110.70
22	BA	1525	A	N9-C4-C5	6.50	108.40	105.80
1	AA	196	A	C5-N7-C8	6.50	107.15	103.90
1	AA	493	A	N9-C4-C5	6.50	108.40	105.80
22	BA	654	A	C4-C5-C6	6.50	120.25	117.00
1	AA	8	A	N9-C4-C5	6.50	108.40	105.80
22	BA	382	A	C4-C5-C6	6.50	120.25	117.00
22	BA	466	A	C4-C5-C6	6.50	120.25	117.00
22	BA	1502	A	N9-C4-C5	6.50	108.40	105.80
22	BA	1698	A	N9-C4-C5	6.50	108.40	105.80
22	BA	2176	A	N9-C4-C5	6.49	108.40	105.80
1	AA	1446	A	C4-C5-C6	6.49	120.25	117.00
1	AA	1229	A	N9-C4-C5	6.49	108.40	105.80
1	AA	1433	A	C4-C5-C6	6.49	120.25	117.00
22	BA	142	A	N9-C4-C5	6.49	108.40	105.80
22	BA	788	A	C4-C5-C6	6.49	120.25	117.00
1	AA	98	A	C4-C5-C6	6.49	120.24	117.00
1	AA	1111	A	C4-C5-C6	6.49	120.25	117.00
22	BA	1069	A	N9-C4-C5	6.49	108.39	105.80
22	BA	1095	A	N9-C4-C5	6.49	108.39	105.80
22	BA	1126	A	C4-C5-C6	6.49	120.24	117.00
22	BA	936	A	C4-C5-C6	6.49	120.24	117.00
22	BA	1237	A	C5-N7-C8	6.49	107.14	103.90
22	BA	1590	A	C4-C5-C6	6.49	120.24	117.00
22	BA	2426	A	N9-C4-C5	6.49	108.39	105.80
22	BA	2614	A	C5-C6-N1	6.49	120.94	117.70
22	BA	262	A	N9-C4-C5	6.48	108.39	105.80
22	BA	2114	A	N3-C4-N9	6.48	132.59	127.40
22	BA	2309	A	C4-C5-C6	6.48	120.24	117.00
1	AA	205	A	N9-C4-C5	6.48	108.39	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	747	A	C5-N7-C8	6.48	107.14	103.90
1	AA	1227	A	C4-C5-C6	6.48	120.24	117.00
1	AA	695	A	C5-N7-C8	6.48	107.14	103.90
22	BA	155	A	N9-C4-C5	6.48	108.39	105.80
22	BA	547	A	N9-C4-C5	6.48	108.39	105.80
1	AA	448	A	N9-C4-C5	6.48	108.39	105.80
22	BA	1899	A	C5-N7-C8	6.48	107.14	103.90
22	BA	2887	A	N9-C4-C5	6.48	108.39	105.80
22	BA	219	A	C4-C5-C6	6.47	120.24	117.00
22	BA	574	A	C4-C5-C6	6.47	120.24	117.00
22	BA	575	A	C4-C5-C6	6.47	120.24	117.00
1	AA	78	A	C5-N7-C8	6.47	107.14	103.90
1	AA	236	A	C5-N7-C8	6.47	107.14	103.90
22	BA	626	A	N9-C4-C5	6.47	108.39	105.80
1	AA	908	A	C4-C5-C6	6.47	120.23	117.00
22	BA	1854	A	N3-C4-N9	6.47	132.58	127.40
1	AA	1080	A	C5-N7-C8	6.47	107.14	103.90
1	AA	1170	A	N3-C4-N9	6.47	132.58	127.40
22	BA	2765	A	C4-C5-C6	6.47	120.23	117.00
1	AA	1447	A	C8-N9-C4	6.47	108.39	105.80
22	BA	2461	A	N3-C4-N9	6.47	132.57	127.40
55	B8	26	A	C8-N9-C4	6.47	108.39	105.80
1	AA	1132	C	C2-N1-C1'	6.47	125.91	118.80
22	BA	6	A	N9-C4-C5	6.47	108.39	105.80
22	BA	478	A	C4-C5-C6	6.47	120.23	117.00
22	BA	1553	A	N3-C4-N9	6.47	132.57	127.40
22	BA	2287	A	N3-C4-N9	6.47	132.57	127.40
22	BA	661	A	N9-C4-C5	6.46	108.39	105.80
22	BA	2792	A	C4-C5-C6	6.46	120.23	117.00
1	AA	461	A	C5-C6-N1	6.46	120.93	117.70
1	AA	968	A	C4-C5-C6	6.46	120.23	117.00
1	AA	181	A	C5-N7-C8	6.46	107.13	103.90
1	AA	1163	A	C5-C6-N1	6.46	120.93	117.70
22	BA	152	A	C5-N7-C8	6.46	107.13	103.90
22	BA	804	A	C4-C5-N7	-6.46	107.47	110.70
22	BA	1744	A	C4-C5-C6	6.46	120.23	117.00
22	BA	2705	A	N9-C4-C5	6.46	108.39	105.80
22	BA	1433	A	N9-C4-C5	6.46	108.38	105.80
22	BA	2287	A	C4-C5-C6	6.46	120.23	117.00
22	BA	2757	A	N3-C4-N9	6.46	132.57	127.40
1	AA	397	A	C5-C6-N1	6.46	120.93	117.70
1	AA	459	A	N7-C8-N9	-6.46	110.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1299	A	C4-C5-C6	6.46	120.23	117.00
23	BB	66	A	C5-N7-C8	6.46	107.13	103.90
1	AA	716	A	C5-N7-C8	6.46	107.13	103.90
1	AA	1171	A	N3-C4-N9	6.46	132.56	127.40
1	AA	1319	A	N3-C4-C5	-6.46	122.28	126.80
1	AA	1476	A	C4-C5-C6	6.46	120.23	117.00
22	BA	2163	A	C4-C5-C6	6.46	120.23	117.00
1	AA	909	A	N9-C4-C5	6.46	108.38	105.80
1	AA	1146	A	C4-C5-C6	6.46	120.23	117.00
22	BA	430	A	C4-C5-C6	6.46	120.23	117.00
22	BA	1496	A	N9-C4-C5	6.46	108.38	105.80
1	AA	715	A	C5-N7-C8	6.45	107.13	103.90
22	BA	2435	A	C4-C5-C6	6.45	120.23	117.00
22	BA	2378	A	N9-C4-C5	6.45	108.38	105.80
1	AA	315	A	N9-C4-C5	6.45	108.38	105.80
3	AC	85	GLU	CA-CB-CG	6.45	127.59	113.40
22	BA	195	A	N7-C8-N9	-6.45	110.57	113.80
1	AA	648	A	N9-C4-C5	6.45	108.38	105.80
1	AA	845	A	N9-C4-C5	6.45	108.38	105.80
22	BA	278	A	N3-C4-N9	6.45	132.56	127.40
22	BA	2147	A	C5-N7-C8	6.45	107.12	103.90
22	BA	2639	A	N9-C4-C5	6.45	108.38	105.80
1	AA	958	A	C4-C5-N7	-6.45	107.48	110.70
22	BA	1089	A	N9-C4-C5	6.45	108.38	105.80
22	BA	1169	A	C4-C5-C6	6.45	120.22	117.00
22	BA	1490	A	C4-C5-C6	6.45	120.22	117.00
22	BA	52	A	N3-C4-N9	6.44	132.56	127.40
1	AA	1176	A	N9-C4-C5	6.44	108.38	105.80
22	BA	219	A	N9-C4-C5	6.44	108.38	105.80
22	BA	272	A	N9-C4-C5	6.44	108.38	105.80
22	BA	2369	A	C4-C5-C6	6.44	120.22	117.00
22	BA	2820	A	C5-N7-C8	6.44	107.12	103.90
1	AA	51	A	N9-C4-C5	6.44	108.38	105.80
22	BA	1877	A	N9-C4-C5	6.44	108.38	105.80
1	AA	329	A	C5-N7-C8	6.44	107.12	103.90
22	BA	941	A	C4-C5-C6	6.44	120.22	117.00
22	BA	730	A	C5-N7-C8	6.44	107.12	103.90
22	BA	2592	G	N3-C4-N9	6.44	129.86	126.00
55	B8	66	A	C4-C5-C6	6.44	120.22	117.00
1	AA	510	A	N9-C4-C5	6.43	108.37	105.80
1	AA	706	A	N9-C4-C5	6.43	108.37	105.80
1	AA	807	A	N9-C4-C5	6.43	108.37	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	231	A	C4-C5-C6	6.43	120.22	117.00
22	BA	1652	A	C4-C5-C6	6.43	120.22	117.00
1	AA	715	A	C4-C5-C6	6.43	120.22	117.00
22	BA	739	A	C5-N7-C8	6.43	107.12	103.90
1	AA	663	A	C4-C5-C6	6.43	120.22	117.00
1	AA	702	A	C5-N7-C8	6.43	107.11	103.90
22	BA	1143	A	C5-N7-C8	6.43	107.11	103.90
22	BA	2734	A	C4-C5-C6	6.43	120.22	117.00
1	AA	728	A	N9-C4-C5	6.43	108.37	105.80
22	BA	415	A	C4-C5-C6	6.43	120.21	117.00
22	BA	2432	A	N9-C4-C5	6.43	108.37	105.80
22	BA	900	A	C4-C5-C6	6.43	120.21	117.00
22	BA	1789	A	C5-N7-C8	6.43	107.11	103.90
22	BA	2478	A	N9-C4-C5	6.43	108.37	105.80
1	AA	1332	A	C5-C6-N1	6.42	120.91	117.70
22	BA	330	A	C4-C5-C6	6.42	120.21	117.00
22	BA	1803	A	C5-N7-C8	6.42	107.11	103.90
22	BA	1960	A	C4-C5-C6	6.42	120.21	117.00
23	BB	46	A	C4-C5-C6	6.42	120.21	117.00
1	AA	780	A	C4-C5-C6	6.42	120.21	117.00
1	AA	923	A	N9-C4-C5	6.42	108.37	105.80
22	BA	278	A	C5-N7-C8	6.42	107.11	103.90
22	BA	443	A	C4-C5-C6	6.42	120.21	117.00
23	BB	57	A	N9-C4-C5	6.42	108.37	105.80
22	BA	1608	A	N3-C4-N9	6.42	132.53	127.40
22	BA	1690	A	C4-C5-C6	6.42	120.21	117.00
22	BA	2482	A	N3-C4-N9	6.42	132.53	127.40
1	AA	246	A	C4-C5-C6	6.42	120.21	117.00
1	AA	749	A	C4-C5-C6	6.42	120.21	117.00
1	AA	1046	A	C5-C6-N1	6.42	120.91	117.70
22	BA	633	A	C5-N7-C8	6.42	107.11	103.90
22	BA	2158	A	N9-C4-C5	6.42	108.37	105.80
22	BA	1230	A	C5-N7-C8	6.42	107.11	103.90
22	BA	471	A	C4-C5-C6	6.41	120.21	117.00
22	BA	538	A	C4-C5-C6	6.41	120.21	117.00
22	BA	1977	A	C4-C5-C6	6.41	120.21	117.00
22	BA	2183	A	N9-C4-C5	6.41	108.36	105.80
1	AA	996	A	C4-C5-N7	-6.41	107.49	110.70
22	BA	1403	A	C5-C6-N1	6.41	120.91	117.70
22	BA	2298	A	C4-C5-C6	6.41	120.21	117.00
1	AA	915	A	N9-C4-C5	6.41	108.36	105.80
22	BA	749	A	N9-C4-C5	6.41	108.36	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2094	A	C4-C5-C6	6.41	120.21	117.00
1	AA	72	A	C5-N7-C8	6.41	107.10	103.90
1	AA	228	A	N9-C4-C5	6.41	108.36	105.80
1	AA	1012	A	N3-C4-N9	6.41	132.53	127.40
1	AA	1305	G	O4'-C1'-N9	6.41	113.33	108.20
22	BA	1260	A	C4-C5-C6	6.41	120.20	117.00
22	BA	1268	A	N9-C4-C5	6.41	108.36	105.80
22	BA	1287	A	N3-C4-N9	6.41	132.53	127.40
1	AA	865	A	N9-C4-C5	6.41	108.36	105.80
1	AA	642	A	N9-C4-C5	6.41	108.36	105.80
22	BA	627	A	N9-C4-C5	6.41	108.36	105.80
22	BA	1928	A	C4-C5-C6	6.41	120.20	117.00
23	BB	39	A	C4-C5-C6	6.41	120.20	117.00
1	AA	1169	A	N9-C4-C5	6.40	108.36	105.80
22	BA	1890	A	C4-C5-N7	-6.40	107.50	110.70
1	AA	1430	A	C4-C5-C6	6.40	120.20	117.00
22	BA	959	A	C8-N9-C4	6.40	108.36	105.80
22	BA	1090	A	C4-C5-C6	6.40	120.20	117.00
22	BA	972	A	C4-C5-C6	6.40	120.20	117.00
22	BA	1953	A	C4-C5-C6	6.40	120.20	117.00
1	AA	1150	A	C4-C5-C6	6.40	120.20	117.00
22	BA	1403	A	N3-C4-N9	6.40	132.52	127.40
22	BA	2311	A	C4-C5-C6	6.40	120.20	117.00
22	BA	2459	A	N3-C4-N9	6.40	132.52	127.40
22	BA	2899	A	C4-C5-C6	6.40	120.20	117.00
1	AA	155	A	C4-C5-C6	6.40	120.20	117.00
22	BA	244	A	N9-C4-C5	6.40	108.36	105.80
22	BA	1175	A	N9-C4-C5	6.40	108.36	105.80
1	AA	1261	A	N9-C4-C5	6.39	108.36	105.80
22	BA	699	A	C4-C5-C6	6.39	120.20	117.00
1	AA	338	A	C5-N7-C8	6.39	107.10	103.90
1	AA	648	A	C4-C5-C6	6.39	120.20	117.00
22	BA	265	A	N9-C4-C5	6.39	108.36	105.80
22	BA	1705	A	N3-C4-N9	6.39	132.51	127.40
22	BA	1039	A	C4-C5-C6	6.39	120.19	117.00
1	AA	161	A	C4-C5-C6	6.39	120.19	117.00
1	AA	746	A	N3-C4-N9	6.39	132.51	127.40
1	AA	923	A	C5-N7-C8	6.39	107.09	103.90
1	AA	174	A	C4-C5-C6	6.39	120.19	117.00
1	AA	673	A	N3-C4-N9	6.39	132.51	127.40
22	BA	1359	A	C5-N7-C8	6.39	107.09	103.90
22	BA	1668	A	C4-C5-N7	-6.39	107.51	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2753	A	C4-C5-C6	6.39	120.19	117.00
1	AA	389	A	C4-C5-C6	6.38	120.19	117.00
1	AA	236	A	N9-C4-C5	6.38	108.35	105.80
1	AA	349	A	N9-C4-C5	6.38	108.35	105.80
1	AA	510	A	C5-N7-C8	6.38	107.09	103.90
1	AA	55	A	N3-C4-N9	6.38	132.50	127.40
1	AA	845	A	C4-C5-C6	6.38	120.19	117.00
23	BB	115	A	C4-C5-C6	6.38	120.19	117.00
1	AA	77	A	N3-C4-N9	6.38	132.50	127.40
1	AA	1299	A	C5-C6-N1	6.38	120.89	117.70
1	AA	3	A	C4-C5-C6	6.38	120.19	117.00
1	AA	116	A	C4-C5-C6	6.38	120.19	117.00
1	AA	1035	A	N9-C4-C5	6.38	108.35	105.80
22	BA	742	A	C4-C5-C6	6.38	120.19	117.00
1	AA	303	A	C4-C5-C6	6.38	120.19	117.00
22	BA	1057	A	N9-C4-C5	6.38	108.35	105.80
22	BA	592	A	C4-C5-C6	6.37	120.19	117.00
22	BA	1284	A	C4-C5-C6	6.37	120.19	117.00
23	BB	50	A	N9-C4-C5	6.37	108.35	105.80
1	AA	487	A	N9-C4-C5	6.37	108.35	105.80
22	BA	161	A	C5-N7-C8	6.37	107.09	103.90
22	BA	1347	A	C4-C5-C6	6.37	120.19	117.00
22	BA	1551	A	C4-C5-N7	-6.37	107.51	110.70
1	AA	892	A	C4-C5-C6	6.37	120.18	117.00
1	AA	1238	A	C4-C5-C6	6.37	120.18	117.00
1	AA	1340	A	C5-C6-N1	6.37	120.88	117.70
22	BA	74	A	C5-N7-C8	6.37	107.08	103.90
22	BA	2062	A	N9-C4-C5	6.37	108.35	105.80
1	AA	1333	A	C4-C5-C6	6.37	120.18	117.00
22	BA	173	A	C4-C5-C6	6.37	120.18	117.00
55	B8	41	A	C5-C6-N1	6.37	120.88	117.70
1	AA	451	A	C4-C5-C6	6.36	120.18	117.00
22	BA	1469	A	N3-C4-N9	6.36	132.49	127.40
22	BA	2173	A	N3-C4-N9	6.36	132.49	127.40
1	AA	533	A	N9-C4-C5	6.36	108.34	105.80
1	AA	892	A	N9-C4-C5	6.36	108.34	105.80
22	BA	599	A	C4-C5-C6	6.36	120.18	117.00
22	BA	1711	A	C4-C5-C6	6.36	120.18	117.00
1	AA	1431	A	C5-N7-C8	6.36	107.08	103.90
22	BA	1365	A	N9-C4-C5	6.36	108.34	105.80
1	AA	250	A	C4-C5-C6	6.36	120.18	117.00
1	AA	595	A	C4-C5-C6	6.36	120.18	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	196	A	N3-C4-N9	6.36	132.49	127.40
22	BA	526	A	C4-C5-C6	6.36	120.18	117.00
22	BA	783	A	C4-C5-N7	-6.36	107.52	110.70
22	BA	1336	A	N9-C4-C5	6.36	108.34	105.80
22	BA	1545	A	C4-C5-C6	6.36	120.18	117.00
22	BA	2042	A	C5-N7-C8	6.36	107.08	103.90
22	BA	508	A	C4-C5-C6	6.35	120.18	117.00
22	BA	793	A	C4-C5-C6	6.35	120.18	117.00
22	BA	118	A	C5-N7-C8	6.35	107.08	103.90
1	AA	533	A	C5-C6-N1	6.35	120.88	117.70
22	BA	2376	A	N9-C4-C5	6.35	108.34	105.80
23	BB	50	A	C4-C5-C6	6.35	120.18	117.00
22	BA	793	A	N3-C4-N9	6.35	132.48	127.40
22	BA	614	A	C4-C5-C6	6.35	120.17	117.00
22	BA	2158	A	C4-C5-C6	6.35	120.17	117.00
1	AA	1256	A	C4-C5-C6	6.35	120.17	117.00
22	BA	1000	A	C5-C6-N1	6.34	120.87	117.70
22	BA	1142	A	N3-C4-N9	6.34	132.48	127.40
22	BA	227	A	C4-C5-C6	6.34	120.17	117.00
22	BA	1669	A	N3-C4-N9	6.34	132.47	127.40
22	BA	1809	A	N9-C4-C5	6.34	108.34	105.80
22	BA	1169	A	N9-C4-C5	6.34	108.34	105.80
22	BA	2766	A	N9-C4-C5	6.34	108.34	105.80
3	AC	88	ARG	CG-CD-NE	6.34	125.11	111.80
22	BA	2101	A	C4-C5-N7	-6.34	107.53	110.70
1	AA	80	A	C5-N7-C8	6.34	107.07	103.90
1	AA	167	A	C4-C5-C6	6.34	120.17	117.00
22	BA	1000	A	C4-C5-N7	-6.34	107.53	110.70
22	BA	2268	A	C4-C5-C6	6.34	120.17	117.00
22	BA	2589	A	C4-C5-N7	-6.34	107.53	110.70
1	AA	1251	A	C4-C5-C6	6.34	120.17	117.00
22	BA	1027	A	C4-C5-C6	6.33	120.17	117.00
22	BA	1046	A	N9-C4-C5	6.33	108.33	105.80
22	BA	1505	A	C4-C5-C6	6.33	120.17	117.00
22	BA	2333	A	C4-C5-C6	6.33	120.17	117.00
22	BA	2634	A	C4-C5-C6	6.33	120.17	117.00
55	B8	20	U	C5-C4-O4	-6.33	122.10	125.90
22	BA	340	A	C4-C5-C6	6.33	120.17	117.00
22	BA	2077	A	C5-N7-C8	6.33	107.07	103.90
22	BA	2682	A	C4-C5-C6	6.33	120.17	117.00
22	BA	1189	A	N9-C4-C5	6.33	108.33	105.80
22	BA	1477	A	C4-C5-C6	6.33	120.17	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2020	A	N9-C4-C5	6.33	108.33	105.80
22	BA	2154	A	N9-C4-C5	6.33	108.33	105.80
23	BB	52	A	C4-C5-C6	6.33	120.17	117.00
22	BA	203	A	C4-C5-C6	6.33	120.16	117.00
22	BA	614	A	N9-C4-C5	6.33	108.33	105.80
22	BA	753	A	N3-C4-N9	6.33	132.46	127.40
22	BA	1048	A	N9-C4-C5	6.33	108.33	105.80
22	BA	1535	A	C4-C5-C6	6.33	120.16	117.00
1	AA	411	A	C8-N9-C4	6.33	108.33	105.80
22	BA	522	A	N3-C4-N9	6.33	132.46	127.40
22	BA	666	A	C4-C5-C6	6.33	120.16	117.00
22	BA	1433	A	C4-C5-C6	6.33	120.16	117.00
22	BA	2054	A	N3-C4-N9	6.33	132.46	127.40
1	AA	496	A	C5-N7-C8	6.32	107.06	103.90
22	BA	637	A	N9-C4-C5	6.32	108.33	105.80
22	BA	981	A	N9-C4-C5	6.32	108.33	105.80
22	BA	1247	A	C4-C5-C6	6.32	120.16	117.00
22	BA	2191	A	C4-C5-C6	6.32	120.16	117.00
1	AA	1428	A	C4-C5-C6	6.32	120.16	117.00
22	BA	1780	A	N9-C4-C5	6.32	108.33	105.80
1	AA	969	A	C4-C5-C6	6.32	120.16	117.00
22	BA	1373	A	N9-C4-C5	6.32	108.33	105.80
1	AA	263	A	C4-C5-C6	6.32	120.16	117.00
22	BA	2176	A	C5-N7-C8	6.32	107.06	103.90
1	AA	160	A	N9-C4-C5	6.32	108.33	105.80
22	BA	443	A	N9-C4-C5	6.32	108.33	105.80
22	BA	1735	A	N9-C4-C5	6.32	108.33	105.80
22	BA	1794	A	C4-C5-C6	6.32	120.16	117.00
22	BA	2478	A	C4-C5-C6	6.32	120.16	117.00
22	BA	2826	A	C4-C5-C6	6.32	120.16	117.00
22	BA	454	A	C4-C5-N7	-6.31	107.54	110.70
22	BA	1287	A	C4-C5-C6	6.31	120.16	117.00
22	BA	2088	A	C4-C5-C6	6.31	120.16	117.00
1	AA	130	A	C4-C5-C6	6.31	120.16	117.00
1	AA	718	A	N3-C4-N9	6.31	132.45	127.40
23	BB	99	A	C4-C5-C6	6.31	120.16	117.00
22	BA	575	A	N9-C4-C5	6.31	108.33	105.80
22	BA	861	A	N3-C4-N9	6.31	132.45	127.40
22	BA	1383	A	N9-C4-C5	6.31	108.33	105.80
22	BA	1679	A	N3-C4-N9	6.31	132.45	127.40
22	BA	2183	A	C4-C5-C6	6.31	120.16	117.00
1	AA	101	A	N9-C4-C5	6.31	108.32	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1022	A	C4-C5-C6	6.31	120.15	117.00
1	AA	1503	A	C4-C5-C6	6.31	120.16	117.00
55	B8	38	A	N3-C4-N9	6.31	132.45	127.40
55	B8	73	A	C8-N9-C4	6.31	108.32	105.80
22	BA	735	A	N3-C4-N9	6.31	132.45	127.40
22	BA	64	A	C4-C5-C6	6.30	120.15	117.00
22	BA	1794	A	N9-C4-C5	6.30	108.32	105.80
22	BA	2879	A	N3-C4-N9	6.30	132.44	127.40
1	AA	195	A	C5-N7-C8	6.30	107.05	103.90
22	BA	2407	A	C5-N7-C8	6.30	107.05	103.90
55	B8	41	A	N3-C4-N9	6.30	132.44	127.40
1	AA	16	A	C4-C5-N7	-6.30	107.55	110.70
1	AA	715	A	N9-C4-C5	6.30	108.32	105.80
1	AA	975	A	C4-C5-C6	6.30	120.15	117.00
22	BA	528	A	C4-C5-C6	6.30	120.15	117.00
22	BA	627	A	C4-C5-C6	6.30	120.15	117.00
22	BA	789	A	N9-C4-C5	6.30	108.32	105.80
22	BA	1029	A	C4-C5-N7	-6.30	107.55	110.70
22	BA	1757	A	C5-N7-C8	6.30	107.05	103.90
22	BA	439	A	C4-C5-C6	6.30	120.15	117.00
22	BA	1151	A	C4-C5-C6	6.30	120.15	117.00
22	BA	1866	A	N9-C4-C5	6.30	108.32	105.80
22	BA	1889	A	C4-C5-C6	6.30	120.15	117.00
1	AA	371	A	C4-C5-N7	-6.30	107.55	110.70
1	AA	901	A	N9-C4-C5	6.30	108.32	105.80
22	BA	91	A	C4-C5-C6	6.30	120.15	117.00
22	BA	1700	A	C4-C5-C6	6.30	120.15	117.00
22	BA	2170	A	C4-C5-C6	6.30	120.15	117.00
1	AA	523	A	N9-C4-C5	6.29	108.32	105.80
22	BA	282	A	C4-C5-C6	6.29	120.15	117.00
22	BA	529	A	C5-N7-C8	6.29	107.05	103.90
22	BA	2682	A	C4-C5-N7	-6.29	107.55	110.70
1	AA	262	A	C4-C5-C6	6.29	120.14	117.00
22	BA	354	A	C4-C5-C6	6.29	120.15	117.00
22	BA	689	A	N3-C4-N9	6.29	132.43	127.40
22	BA	1978	A	N3-C4-N9	6.29	132.43	127.40
1	AA	167	A	N9-C4-C5	6.29	108.32	105.80
1	AA	325	A	N9-C4-C5	6.29	108.32	105.80
1	AA	743	A	N9-C4-C5	6.29	108.32	105.80
22	BA	2851	A	C4-C5-C6	6.29	120.14	117.00
22	BA	844	A	N9-C4-C5	6.29	108.31	105.80
22	BA	933	A	C4-C5-C6	6.29	120.14	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	430	A	N9-C4-C5	6.29	108.31	105.80
22	BA	2407	A	N3-C4-N9	6.29	132.43	127.40
22	BA	5	A	N3-C4-N9	6.28	132.43	127.40
22	BA	368	A	N9-C4-C5	6.28	108.31	105.80
22	BA	1598	A	C4-C5-C6	6.28	120.14	117.00
22	BA	1787	A	N9-C4-C5	6.28	108.31	105.80
22	BA	371	A	N9-C4-C5	6.28	108.31	105.80
22	BA	1614	A	C5-N7-C8	6.28	107.04	103.90
22	BA	2090	A	N3-C4-N9	6.28	132.43	127.40
22	BA	2273	A	N3-C4-N9	6.28	132.43	127.40
22	BA	2635	A	C4-C5-C6	6.28	120.14	117.00
22	BA	1403	A	N9-C4-C5	6.28	108.31	105.80
22	BA	1711	A	N9-C4-C5	6.28	108.31	105.80
22	BA	1858	A	C4-C5-C6	6.28	120.14	117.00
1	AA	814	A	N9-C4-C5	6.28	108.31	105.80
22	BA	173	A	N9-C4-C5	6.28	108.31	105.80
1	AA	502	A	N3-C4-N9	6.27	132.42	127.40
22	BA	1551	A	C4-C5-C6	6.27	120.14	117.00
22	BA	255	A	N3-C4-N9	6.27	132.42	127.40
22	BA	1754	A	C5-N7-C8	6.27	107.04	103.90
22	BA	2126	A	N9-C4-C5	6.27	108.31	105.80
22	BA	2412	A	N9-C4-C5	6.27	108.31	105.80
23	BB	53	A	C4-C5-C6	6.27	120.14	117.00
1	AA	329	A	N9-C4-C5	6.27	108.31	105.80
1	AA	1246	A	C4-C5-C6	6.27	120.14	117.00
22	BA	21	A	N9-C4-C5	6.27	108.31	105.80
22	BA	213	A	N9-C4-C5	6.27	108.31	105.80
22	BA	2564	A	N9-C4-C5	6.27	108.31	105.80
22	BA	2738	A	N9-C4-C5	6.27	108.31	105.80
1	AA	313	A	C4-C5-C6	6.27	120.13	117.00
22	BA	1597	A	C4-C5-N7	-6.27	107.57	110.70
22	BA	1872	A	N3-C4-N9	6.27	132.41	127.40
1	AA	563	A	C5-N7-C8	6.26	107.03	103.90
1	AA	596	A	N9-C4-C5	6.26	108.31	105.80
22	BA	1098	A	N3-C4-N9	6.26	132.41	127.40
22	BA	1276	A	N9-C4-C5	6.26	108.31	105.80
1	AA	50	A	N9-C4-C5	6.26	108.31	105.80
1	AA	228	A	C4-C5-C6	6.26	120.13	117.00
1	AA	807	A	C4-C5-C6	6.26	120.13	117.00
22	BA	1027	A	C5-N7-C8	6.26	107.03	103.90
55	B8	26	A	N3-C4-N9	6.26	132.41	127.40
22	BA	449	A	N3-C4-N9	6.26	132.41	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	718	A	N9-C4-C5	6.26	108.30	105.80
22	BA	1919	A	N9-C4-C5	6.26	108.31	105.80
22	BA	2813	A	C5-N7-C8	6.26	107.03	103.90
1	AA	363	A	C4-C5-C6	6.26	120.13	117.00
1	AA	831	A	C4-C5-C6	6.26	120.13	117.00
22	BA	2273	A	C4-C5-C6	6.26	120.13	117.00
22	BA	2378	A	C5-N7-C8	6.26	107.03	103.90
22	BA	1866	A	C5-N7-C8	6.26	107.03	103.90
22	BA	2369	A	N9-C4-C5	6.26	108.30	105.80
1	AA	116	A	N9-C4-C5	6.26	108.30	105.80
1	AA	794	A	C4-C5-C6	6.26	120.13	117.00
22	BA	470	A	C5-N7-C8	6.26	107.03	103.90
22	BA	689	A	C4-C5-N7	-6.26	107.57	110.70
22	BA	1701	A	C4-C5-C6	6.26	120.13	117.00
22	BA	1889	A	C4-C5-N7	-6.26	107.57	110.70
1	AA	560	A	N9-C4-C5	6.25	108.30	105.80
1	AA	790	A	N9-C4-C5	6.25	108.30	105.80
22	BA	1067	A	C4-C5-C6	6.25	120.13	117.00
1	AA	1280	A	C4-C5-C6	6.25	120.13	117.00
22	BA	1515	A	C5-N7-C8	6.25	107.03	103.90
22	BA	2809	A	C4-C5-C6	6.25	120.13	117.00
22	BA	374	A	N9-C4-C5	6.25	108.30	105.80
22	BA	1384	A	C4-C5-C6	6.25	120.12	117.00
1	AA	28	A	C5-N7-C8	6.25	107.02	103.90
1	AA	1005	A	C4-C5-C6	6.25	120.12	117.00
22	BA	2670	A	N9-C4-C5	6.25	108.30	105.80
22	BA	742	A	N9-C4-C5	6.25	108.30	105.80
22	BA	2247	A	N3-C4-N9	6.25	132.40	127.40
22	BA	1226	A	N9-C4-C5	6.24	108.30	105.80
22	BA	1544	A	C4-C5-C6	6.24	120.12	117.00
22	BA	2425	A	N9-C4-C5	6.24	108.30	105.80
22	BA	391	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1919	A	C5-N7-C8	6.24	107.02	103.90
22	BA	2820	A	N9-C4-C5	6.24	108.30	105.80
1	AA	781	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1434	A	C4-C5-N7	-6.24	107.58	110.70
22	BA	216	A	C4-C5-N7	-6.24	107.58	110.70
22	BA	825	A	C4-C5-N7	-6.24	107.58	110.70
22	BA	2278	A	N9-C4-C5	6.24	108.30	105.80
22	BA	2322	A	N9-C4-C5	6.24	108.30	105.80
1	AA	712	A	N3-C4-N9	6.24	132.39	127.40
1	AA	1151	A	N9-C4-C5	6.24	108.30	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	227	A	N9-C4-C5	6.24	108.30	105.80
22	BA	1096	A	C4-C5-C6	6.24	120.12	117.00
2	AB	18	HIS	CB-CA-C	6.24	122.87	110.40
1	AA	412	A	C5-C6-N1	6.24	120.82	117.70
22	BA	311	A	C4-C5-C6	6.24	120.12	117.00
22	BA	2322	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1175	A	C4-C5-C6	6.23	120.12	117.00
22	BA	1205	A	C4-C5-N7	-6.23	107.58	110.70
1	AA	716	A	N9-C4-C5	6.23	108.29	105.80
22	BA	925	A	C4-C5-C6	6.23	120.12	117.00
22	BA	2778	A	C4-C5-C6	6.23	120.12	117.00
22	BA	91	A	N9-C4-C5	6.23	108.29	105.80
22	BA	1665	A	C4-C5-C6	6.23	120.11	117.00
22	BA	2541	A	N9-C4-C5	6.23	108.29	105.80
22	BA	2560	A	C4-C5-C6	6.23	120.11	117.00
23	BB	73	A	N3-C4-N9	6.23	132.38	127.40
1	AA	1197	A	C5-N7-C8	6.22	107.01	103.90
22	BA	89	A	C4-C5-C6	6.22	120.11	117.00
22	BA	95	A	N9-C4-C5	6.22	108.29	105.80
22	BA	345	A	N9-C4-C5	6.22	108.29	105.80
55	B8	19	G	OP2-P-O3'	-6.22	91.50	105.20
22	BA	131	A	N9-C4-C5	6.22	108.29	105.80
22	BA	1151	A	N3-C4-N9	6.22	132.38	127.40
22	BA	1762	A	C4-C5-C6	6.22	120.11	117.00
22	BA	2635	A	N3-C4-N9	6.22	132.38	127.40
23	BB	108	A	C4-C5-C6	6.22	120.11	117.00
22	BA	829	A	C5-N7-C8	6.22	107.01	103.90
22	BA	1952	A	C4-C5-C6	6.22	120.11	117.00
22	BA	2654	A	C4-C5-C6	6.22	120.11	117.00
22	BA	2856	A	N9-C4-C5	6.22	108.29	105.80
23	BB	34	A	N9-C4-C5	6.22	108.29	105.80
22	BA	21	A	N3-C4-N9	6.22	132.38	127.40
22	BA	300	A	N9-C4-C5	6.22	108.29	105.80
22	BA	905	A	C4-C5-N7	-6.22	107.59	110.70
22	BA	2281	A	C4-C5-N7	-6.21	107.59	110.70
1	AA	327	A	C4-C5-C6	6.21	120.11	117.00
1	AA	408	A	C4-C5-C6	6.21	120.11	117.00
1	AA	1274	A	N9-C4-C5	6.21	108.28	105.80
22	BA	404	A	N9-C4-C5	6.21	108.28	105.80
22	BA	497	A	C4-C5-C6	6.21	120.11	117.00
22	BA	592	A	N3-C4-N9	6.21	132.37	127.40
22	BA	2426	A	C4-C5-C6	6.21	120.11	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2632	A	N9-C4-C5	6.21	108.28	105.80
1	AA	1004	A	C5-C6-N1	6.21	120.80	117.70
22	BA	1571	A	N3-C4-N9	6.21	132.37	127.40
23	BB	101	A	C6-N1-C2	-6.21	114.88	118.60
1	AA	1340	A	C5-N7-C8	6.21	107.00	103.90
22	BA	470	A	N3-C4-N9	6.21	132.37	127.40
22	BA	1336	A	C4-C5-C6	6.21	120.10	117.00
22	BA	1354	A	N9-C4-C5	6.21	108.28	105.80
22	BA	1134	A	C5-N7-C8	6.21	107.00	103.90
22	BA	1739	A	C4-C5-C6	6.21	120.10	117.00
22	BA	507	A	N9-C4-C5	6.20	108.28	105.80
23	BB	109	A	C4-C5-C6	6.20	120.10	117.00
1	AA	53	A	N9-C4-C5	6.20	108.28	105.80
1	AA	978	A	C4-C5-N7	-6.20	107.60	110.70
22	BA	176	A	N3-C4-N9	6.20	132.36	127.40
22	BA	1085	A	C4-C5-C6	6.20	120.10	117.00
22	BA	2665	A	N9-C4-C5	6.20	108.28	105.80
1	AA	139	A	C4-C5-C6	6.20	120.10	117.00
1	AA	189	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1196	A	N9-C4-C5	6.20	108.28	105.80
22	BA	21	A	C5-C6-N1	6.20	120.80	117.70
22	BA	1532	A	C4-C5-C6	6.20	120.10	117.00
22	BA	2600	A	C5-N7-C8	6.20	107.00	103.90
22	BA	541	A	C4-C5-C6	6.20	120.10	117.00
22	BA	563	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1171	A	N9-C4-C5	6.20	108.28	105.80
22	BA	927	A	C4-C5-C6	6.20	120.10	117.00
22	BA	983	A	C4-C5-C6	6.20	120.10	117.00
22	BA	2080	A	N3-C4-N9	6.20	132.36	127.40
22	BA	2764	A	C4-C5-N7	-6.20	107.60	110.70
22	BA	2336	A	C4-C5-C6	6.19	120.10	117.00
22	BA	2590	A	N9-C4-C5	6.19	108.28	105.80
1	AA	155	A	N9-C4-C5	6.19	108.28	105.80
1	AA	478	A	N9-C4-C5	6.19	108.28	105.80
22	BA	161	A	C4-C5-C6	6.19	120.10	117.00
22	BA	412	A	C5-N7-C8	6.19	107.00	103.90
22	BA	670	A	N9-C4-C5	6.19	108.28	105.80
22	BA	899	A	C4-C5-C6	6.19	120.10	117.00
22	BA	1129	A	N9-C4-C5	6.19	108.28	105.80
23	BB	99	A	N9-C4-C5	6.19	108.28	105.80
1	AA	364	A	C4-C5-C6	6.19	120.09	117.00
22	BA	402	A	C4-C5-C6	6.19	120.09	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1096	A	N9-C4-C5	6.19	108.28	105.80
22	BA	1913	A	C4-C5-C6	6.19	120.10	117.00
22	BA	401	A	N9-C4-C5	6.19	108.28	105.80
22	BA	1801	A	C5-N7-C8	6.19	106.99	103.90
1	AA	706	A	N3-C4-N9	6.19	132.35	127.40
1	AA	573	A	N9-C4-C5	6.18	108.27	105.80
1	AA	1288	A	C4-C5-C6	6.18	120.09	117.00
22	BA	221	A	C5-N7-C8	6.18	106.99	103.90
22	BA	1373	A	C5-N7-C8	6.18	106.99	103.90
22	BA	2868	A	N9-C4-C5	6.18	108.27	105.80
1	AA	1191	A	N9-C4-C5	6.18	108.27	105.80
22	BA	2776	A	C4-C5-N7	-6.18	107.61	110.70
22	BA	2518	A	C8-N9-C4	6.18	108.27	105.80
22	BA	2583	G	N1-C6-O6	-6.18	116.19	119.90
22	BA	346	A	N9-C4-C5	6.18	108.27	105.80
22	BA	941	A	C4-C5-N7	-6.18	107.61	110.70
22	BA	1270	C	C6-N1-C2	-6.18	117.83	120.30
1	AA	1014	A	C4-C5-C6	6.17	120.09	117.00
22	BA	820	A	C4-C5-N7	-6.17	107.61	110.70
22	BA	2336	A	N9-C4-C5	6.17	108.27	105.80
23	BB	66	A	N9-C4-C5	6.17	108.27	105.80
1	AA	608	A	N9-C4-C5	6.17	108.27	105.80
1	AA	872	A	C4-C5-C6	6.17	120.09	117.00
1	AA	1418	A	N3-C4-N9	6.17	132.34	127.40
22	BA	1054	A	N9-C4-C5	6.17	108.27	105.80
22	BA	2054	A	C4-C5-C6	6.17	120.09	117.00
22	BA	21	A	C4-C5-C6	6.17	120.08	117.00
22	BA	2058	A	N9-C4-C5	6.17	108.27	105.80
22	BA	56	A	N9-C4-C5	6.17	108.27	105.80
22	BA	2009	A	C4-C5-C6	6.17	120.08	117.00
22	BA	2059	A	C4-C5-C6	6.17	120.08	117.00
1	AA	1446	A	C4-C5-N7	-6.17	107.62	110.70
22	BA	2800	A	N9-C4-C5	6.17	108.27	105.80
1	AA	459	A	N9-C4-C5	6.17	108.27	105.80
1	AA	1410	A	C4-C5-C6	6.17	120.08	117.00
22	BA	2134	A	C4-C5-C6	6.17	120.08	117.00
1	AA	1468	A	N3-C4-N9	6.16	132.33	127.40
22	BA	2377	A	N9-C4-C5	6.16	108.27	105.80
1	AA	1398	A	C4-C5-C6	6.16	120.08	117.00
22	BA	477	A	N3-C4-N9	6.16	132.33	127.40
22	BA	996	A	N3-C4-N9	6.16	132.33	127.40
22	BA	1143	A	N3-C4-N9	6.16	132.33	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2346	A	C4-C5-C6	6.16	120.08	117.00
1	AA	72	A	N9-C4-C5	6.16	108.26	105.80
1	AA	1197	A	N3-C4-N9	6.16	132.33	127.40
22	BA	1598	A	N3-C4-N9	6.16	132.33	127.40
1	AA	1042	A	C4-C5-C6	6.16	120.08	117.00
22	BA	1998	A	N3-C4-N9	6.16	132.33	127.40
22	BA	1757	A	C4-C5-C6	6.16	120.08	117.00
22	BA	2020	A	C5-C6-N1	6.16	120.78	117.70
22	BA	479	A	C4-C5-N7	-6.15	107.62	110.70
22	BA	1722	A	N9-C4-C5	6.15	108.26	105.80
1	AA	1363	A	N3-C4-N9	6.15	132.32	127.40
22	BA	146	A	N9-C4-C5	6.15	108.26	105.80
22	BA	1048	A	N3-C4-N9	6.15	132.32	127.40
22	BA	1226	A	C4-C5-C6	6.15	120.08	117.00
1	AA	766	A	C4-C5-C6	6.15	120.08	117.00
22	BA	1532	A	N9-C4-C5	6.15	108.26	105.80
22	BA	2541	A	C5-C6-N1	6.15	120.77	117.70
22	BA	126	A	C5-N7-C8	6.15	106.97	103.90
22	BA	556	A	C4-C5-C6	6.15	120.07	117.00
22	BA	2453	A	C4-C5-C6	6.15	120.07	117.00
1	AA	152	A	C5-N7-C8	6.15	106.97	103.90
22	BA	14	A	C4-C5-C6	6.15	120.07	117.00
1	AA	553	A	C5-C6-N1	6.14	120.77	117.70
1	AA	1357	A	N9-C4-C5	6.14	108.26	105.80
4	AD	33	LYS	CD-CE-NZ	-6.14	97.57	111.70
22	BA	592	A	N9-C4-C5	6.14	108.26	105.80
22	BA	2634	A	N3-C4-N9	6.14	132.31	127.40
1	AA	71	A	C4-C5-C6	6.14	120.07	117.00
22	BA	454	A	C4-C5-C6	6.14	120.07	117.00
22	BA	819	A	N9-C4-C5	6.14	108.26	105.80
1	AA	583	A	C4-C5-N7	-6.14	107.63	110.70
22	BA	415	A	N3-C4-N9	6.14	132.31	127.40
22	BA	705	A	N9-C4-C5	6.14	108.26	105.80
22	BA	896	A	C4-C5-C6	6.14	120.07	117.00
22	BA	1938	A	N9-C4-C5	6.14	108.26	105.80
1	AA	1219	A	N9-C4-C5	6.14	108.25	105.80
13	AM	42	ASP	CB-CG-OD1	6.14	123.82	118.30
22	BA	244	A	N3-C4-N9	6.14	132.31	127.40
22	BA	1713	A	N9-C4-C5	6.14	108.25	105.80
22	BA	547	A	C4-C5-C6	6.13	120.07	117.00
22	BA	2077	A	N3-C4-N9	6.13	132.31	127.40
22	BA	685	A	C5-C6-N1	6.13	120.77	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1142	A	C5-C6-N1	6.13	120.77	117.70
1	AA	1158	C	C2-N1-C1'	6.13	125.55	118.80
1	AA	1433	A	N9-C4-C5	6.13	108.25	105.80
22	BA	1127	A	C4-C5-C6	6.13	120.07	117.00
22	BA	1829	A	N9-C4-C5	6.13	108.25	105.80
22	BA	2108	A	C5-N7-C8	6.13	106.97	103.90
1	AA	279	A	C5-N7-C8	6.13	106.97	103.90
22	BA	2097	A	N3-C4-N9	6.13	132.30	127.40
22	BA	1672	A	C4-C5-C6	6.13	120.06	117.00
1	AA	1146	A	N9-C4-C5	6.13	108.25	105.80
1	AA	1306	A	N9-C4-C5	6.13	108.25	105.80
1	AA	1374	A	N9-C4-C5	6.13	108.25	105.80
22	BA	213	A	C5-C6-N1	6.13	120.76	117.70
1	AA	32	A	N9-C4-C5	6.12	108.25	105.80
1	AA	498	A	C5-C6-N6	6.12	128.60	123.70
22	BA	2518	A	C4-C5-C6	6.12	120.06	117.00
22	BA	1786	A	C4-C5-N7	-6.12	107.64	110.70
1	AA	344	A	C4-C5-C6	6.12	120.06	117.00
1	AA	977	A	N3-C4-N9	6.12	132.30	127.40
22	BA	782	A	C5-C6-N1	6.12	120.76	117.70
1	AA	1016	A	C4-C5-C6	6.12	120.06	117.00
22	BA	1302	A	C4-C5-C6	6.12	120.06	117.00
22	BA	1469	A	N9-C4-C5	6.12	108.25	105.80
1	AA	181	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1167	A	N9-C4-C5	6.12	108.25	105.80
22	BA	783	A	N3-C4-N9	6.12	132.29	127.40
23	BB	119	A	N9-C4-C5	6.12	108.25	105.80
1	AA	2	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1191	A	N3-C4-N9	6.12	132.29	127.40
1	AA	1238	A	C4-C5-N7	-6.12	107.64	110.70
22	BA	514	A	N9-C4-C5	6.12	108.25	105.80
1	AA	1155	A	C4-C5-C6	6.11	120.06	117.00
22	BA	482	A	N9-C4-C5	6.11	108.25	105.80
22	BA	1385	A	N9-C4-C5	6.11	108.25	105.80
22	BA	471	A	N9-C4-C5	6.11	108.25	105.80
22	BA	2670	A	C4-C5-C6	6.11	120.06	117.00
22	BA	2826	A	C4-C5-N7	-6.11	107.64	110.70
55	B8	42	A	N3-C4-N9	6.11	132.29	127.40
22	BA	582	A	N3-C4-N9	6.11	132.29	127.40
22	BA	633	A	C4-C5-C6	6.11	120.06	117.00
1	AA	288	A	N9-C4-C5	6.11	108.24	105.80
22	BA	422	A	C4-C5-N7	-6.11	107.64	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2451	A	N7-C8-N9	-6.11	110.75	113.80
1	AA	320	A	C4-C5-N7	-6.11	107.65	110.70
22	BA	28	A	C4-C5-C6	6.11	120.05	117.00
22	BA	1630	A	C4-C5-N7	-6.11	107.65	110.70
22	BA	2448	A	C5-N7-C8	6.11	106.95	103.90
1	AA	553	A	N3-C4-N9	6.11	132.28	127.40
1	AA	1287	A	C4-C5-C6	6.11	120.05	117.00
22	BA	203	A	C4-C5-N7	-6.11	107.65	110.70
22	BA	391	A	N3-C4-N9	6.11	132.28	127.40
55	B8	42	A	C8-N9-C4	6.11	108.24	105.80
22	BA	501	A	N9-C4-C5	6.10	108.24	105.80
1	AA	250	A	N9-C4-C5	6.10	108.24	105.80
22	BA	241	A	C4-C5-N7	-6.10	107.65	110.70
22	BA	2602	A	N9-C4-C5	6.10	108.24	105.80
1	AA	673	A	C5-C6-N1	6.10	120.75	117.70
22	BA	1655	A	N9-C4-C5	6.10	108.24	105.80
22	BA	2287	A	C8-N9-C4	6.10	108.24	105.80
22	BA	2868	A	N3-C4-N9	6.10	132.28	127.40
22	BA	429	A	C4-C5-C6	6.10	120.05	117.00
22	BA	675	A	C4-C5-N7	-6.10	107.65	110.70
22	BA	677	A	C5-C6-N1	6.10	120.75	117.70
22	BA	820	A	N3-C4-N9	6.10	132.28	127.40
22	BA	2566	A	N9-C4-C5	6.10	108.24	105.80
22	BA	2749	A	C5-N7-C8	6.10	106.95	103.90
22	BA	2750	A	N9-C4-C5	6.10	108.24	105.80
1	AA	1492	A	C4-C5-C6	6.10	120.05	117.00
22	BA	515	A	C4-C5-N7	-6.10	107.65	110.70
22	BA	1590	A	N9-C4-C5	6.10	108.24	105.80
22	BA	1744	A	N9-C4-C5	6.10	108.24	105.80
1	AA	1275	A	N9-C4-C5	6.09	108.24	105.80
22	BA	1336	A	N3-C4-N9	6.09	132.28	127.40
22	BA	1597	A	C4-C5-C6	6.09	120.05	117.00
22	BA	1077	A	C4-C5-C6	6.09	120.05	117.00
22	BA	1244	A	C5-C6-N1	6.09	120.75	117.70
22	BA	1746	A	N9-C4-C5	6.09	108.24	105.80
23	BB	104	A	N9-C4-C5	6.09	108.24	105.80
1	AA	131	A	C4-C5-C6	6.09	120.04	117.00
22	BA	1276	A	N3-C4-N9	6.09	132.27	127.40
1	AA	1179	A	C4-C5-C6	6.09	120.04	117.00
1	AA	1437	A	C4-C5-C6	6.09	120.04	117.00
22	BA	1966	A	C4-C5-C6	6.09	120.04	117.00
22	BA	2170	A	N9-C4-C5	6.09	108.23	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	750	A	C4-C5-C6	6.08	120.04	117.00
22	BA	423	A	C4-C5-N7	-6.08	107.66	110.70
1	AA	65	A	C4-C5-C6	6.08	120.04	117.00
1	AA	306	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1271	A	N9-C4-C5	6.08	108.23	105.80
22	BA	320	A	C4-C5-C6	6.08	120.04	117.00
22	BA	800	A	C4-C5-C6	6.08	120.04	117.00
22	BA	936	A	N9-C4-C5	6.08	108.23	105.80
22	BA	2211	A	C4-C5-C6	6.08	120.04	117.00
22	BA	892	A	C4-C5-C6	6.08	120.04	117.00
22	BA	1133	A	C5-N7-C8	6.08	106.94	103.90
22	BA	1610	A	N9-C4-C5	6.08	108.23	105.80
22	BA	2042	A	C4-C5-C6	6.08	120.04	117.00
22	BA	2212	A	C4-C5-C6	6.08	120.04	117.00
1	AA	559	A	N9-C4-C5	6.08	108.23	105.80
1	AA	747	A	C4-C5-C6	6.08	120.04	117.00
1	AA	574	A	N9-C4-C5	6.07	108.23	105.80
1	AA	977	A	N9-C4-C5	6.07	108.23	105.80
1	AA	1229	A	C4-C5-C6	6.07	120.04	117.00
22	BA	644	A	N3-C4-N9	6.07	132.26	127.40
22	BA	2000	C	N1-C2-O2	6.07	122.54	118.90
22	BA	2340	A	N3-C4-N9	6.07	132.26	127.40
1	AA	496	A	C4-C5-C6	6.07	120.03	117.00
1	AA	1021	A	C4-C5-C6	6.07	120.04	117.00
22	BA	753	A	N9-C4-C5	6.07	108.23	105.80
22	BA	2634	A	N9-C4-C5	6.07	108.23	105.80
22	BA	83	A	C4-C5-C6	6.07	120.03	117.00
22	BA	792	A	N3-C4-N9	6.07	132.25	127.40
22	BA	947	A	N3-C4-N9	6.07	132.25	127.40
22	BA	2711	A	C4-C5-C6	6.07	120.03	117.00
1	AA	101	A	N3-C4-N9	6.07	132.25	127.40
1	AA	320	A	C4-C5-C6	6.07	120.03	117.00
1	AA	923	A	N3-C4-N9	6.07	132.25	127.40
22	BA	2009	A	N9-C4-C5	6.07	108.23	105.80
22	BA	2572	A	C4-C5-N7	-6.07	107.67	110.70
1	AA	253	A	C8-N9-C4	6.07	108.23	105.80
1	AA	279	A	C4-C5-C6	6.07	120.03	117.00
1	AA	300	A	C5-N7-C8	6.07	106.93	103.90
22	BA	632	A	N9-C4-C5	6.07	108.23	105.80
22	BA	734	A	C4-C5-C6	6.07	120.03	117.00
23	BB	15	A	C5-N7-C8	6.07	106.93	103.90
23	BB	104	A	C4-C5-C6	6.07	120.03	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	716	A	N9-C4-C5	6.06	108.23	105.80
22	BA	1616	A	C4-C5-C6	6.06	120.03	117.00
1	AA	53	A	C4-C5-C6	6.06	120.03	117.00
22	BA	460	A	C4-C5-C6	6.06	120.03	117.00
22	BA	1978	A	C4-C5-C6	6.06	120.03	117.00
22	BA	2077	A	N9-C4-C5	6.06	108.22	105.80
22	BA	2883	A	C4-C5-C6	6.06	120.03	117.00
1	AA	116	A	N3-C4-N9	6.06	132.25	127.40
1	AA	1441	A	C4-C5-C6	6.06	120.03	117.00
22	BA	727	A	C4-C5-C6	6.06	120.03	117.00
22	BA	1495	A	C4-C5-C6	6.06	120.03	117.00
22	BA	2741	A	C4-C5-N7	-6.06	107.67	110.70
22	BA	2813	A	N3-C4-N9	6.06	132.25	127.40
1	AA	1021	A	N9-C4-C5	6.06	108.22	105.80
22	BA	311	A	N9-C4-C5	6.06	108.22	105.80
22	BA	979	A	C4-C5-C6	6.06	120.03	117.00
55	B8	14	A	N3-C4-N9	6.06	132.25	127.40
22	BA	49	A	N9-C4-C5	6.06	108.22	105.80
22	BA	599	A	N9-C4-C5	6.06	108.22	105.80
22	BA	2799	A	C5-N7-C8	6.06	106.93	103.90
22	BA	925	A	N9-C4-C5	6.05	108.22	105.80
22	BA	1147	A	N9-C4-C5	6.05	108.22	105.80
22	BA	2199	A	C4-C5-C6	6.05	120.03	117.00
1	AA	675	A	C4-C5-C6	6.05	120.02	117.00
1	AA	681	A	N9-C4-C5	6.05	108.22	105.80
1	AA	906	A	C4-C5-C6	6.05	120.03	117.00
1	AA	1507	A	C4-C5-C6	6.05	120.03	117.00
22	BA	1286	A	C4-C5-N7	-6.05	107.68	110.70
23	BB	119	A	C4-C5-C6	6.05	120.03	117.00
1	AA	246	A	N9-C4-C5	6.05	108.22	105.80
22	BA	1899	A	C4-C5-C6	6.05	120.02	117.00
1	AA	315	A	C4-C5-C6	6.04	120.02	117.00
22	BA	146	A	C4-C5-C6	6.04	120.02	117.00
1	AA	270	A	N9-C4-C5	6.04	108.22	105.80
1	AA	1269	A	C4-C5-C6	6.04	120.02	117.00
22	BA	1420	A	C4-C5-C6	6.04	120.02	117.00
1	AA	495	A	N9-C4-C5	6.04	108.22	105.80
22	BA	538	A	N9-C4-C5	6.04	108.22	105.80
1	AA	1413	A	C4-C5-C6	6.04	120.02	117.00
22	BA	270	A	C4-C5-C6	6.04	120.02	117.00
22	BA	453	A	N3-C4-N9	6.04	132.23	127.40
22	BA	478	A	C4-C5-N7	-6.04	107.68	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2171	A	N9-C4-C5	6.04	108.22	105.80
22	BA	2449	U	N1-C2-N3	6.04	118.52	114.90
55	B8	21	A	N3-C4-N9	6.04	132.23	127.40
22	BA	2003	A	C4-C5-C6	6.04	120.02	117.00
22	BA	2589	A	C4-C5-C6	6.04	120.02	117.00
22	BA	2703	C	C6-N1-C2	-6.04	117.89	120.30
23	BB	34	A	C4-C5-C6	6.04	120.02	117.00
55	B8	26	A	C5-C6-N1	6.04	120.72	117.70
1	AA	309	A	N9-C4-C5	6.03	108.21	105.80
1	AA	712	A	N9-C4-C5	6.03	108.21	105.80
1	AA	1167	A	C4-C5-C6	6.03	120.02	117.00
1	AA	1201	A	N9-C4-C5	6.03	108.21	105.80
1	AA	1375	A	N9-C4-C5	6.03	108.21	105.80
22	BA	802	A	N9-C4-C5	6.03	108.21	105.80
22	BA	1213	A	N9-C4-C5	6.03	108.21	105.80
1	AA	1311	A	C4-C5-C6	6.03	120.02	117.00
22	BA	1230	A	C4-C5-C6	6.03	120.02	117.00
22	BA	2497	A	C4-C5-N7	-6.03	107.69	110.70
1	AA	878	A	C4-C5-C6	6.03	120.01	117.00
22	BA	654	A	N9-C4-C5	6.03	108.21	105.80
22	BA	1932	A	N9-C4-C5	6.03	108.21	105.80
22	BA	2082	A	N9-C4-C5	6.03	108.21	105.80
22	BA	2565	A	N9-C4-C5	6.03	108.21	105.80
1	AA	432	A	N9-C4-C5	6.02	108.21	105.80
1	AA	946	A	N3-C4-N9	6.02	132.22	127.40
1	AA	1431	A	C4-C5-C6	6.02	120.01	117.00
22	BA	1254	A	C4-C5-C6	6.02	120.01	117.00
22	BA	2753	A	C4-C5-N7	-6.02	107.69	110.70
22	BA	1784	A	C4-C5-C6	6.02	120.01	117.00
22	BA	655	A	N9-C4-C5	6.02	108.21	105.80
1	AA	1480	A	C4-C5-C6	6.02	120.01	117.00
22	BA	73	A	N9-C4-C5	6.02	108.21	105.80
22	BA	1549	A	N9-C4-C5	6.02	108.21	105.80
22	BA	1689	A	N9-C4-C5	6.02	108.21	105.80
1	AA	65	A	N9-C4-C5	6.01	108.21	105.80
1	AA	109	A	C4-C5-C6	6.01	120.01	117.00
1	AA	349	A	C4-C5-C6	6.01	120.01	117.00
1	AA	1092	A	C4-C5-C6	6.01	120.01	117.00
22	BA	156	A	N9-C4-C5	6.01	108.21	105.80
1	AA	1082	A	N9-C4-C5	6.01	108.20	105.80
1	AA	356	A	N3-C4-N9	6.01	132.21	127.40
22	BA	447	A	N9-C4-C5	6.01	108.20	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	609	A	N9-C4-C5	6.01	108.20	105.80
1	AA	59	A	C4-C5-C6	6.01	120.00	117.00
22	BA	322	A	C4-C5-N7	-6.01	107.69	110.70
22	BA	1549	A	N3-C4-N9	6.01	132.21	127.40
1	AA	908	A	N9-C4-C5	6.01	108.20	105.80
22	BA	262	A	C5-C6-N1	6.01	120.70	117.70
1	AA	1	A	N9-C4-C5	6.00	108.20	105.80
22	BA	616	A	N3-C4-N9	6.00	132.20	127.40
23	BB	52	A	N9-C4-C5	6.00	108.20	105.80
55	B8	69	A	N3-C4-N9	6.00	132.20	127.40
1	AA	946	A	N9-C4-C5	6.00	108.20	105.80
22	BA	608	A	N3-C4-N9	6.00	132.20	127.40
1	AA	460	A	C5-N7-C8	6.00	106.90	103.90
1	AA	743	A	N3-C4-N9	6.00	132.20	127.40
1	AA	938	A	C5-C6-N1	6.00	120.70	117.70
22	BA	472	A	N9-C4-C5	6.00	108.20	105.80
22	BA	633	A	N9-C4-C5	6.00	108.20	105.80
22	BA	829	A	N9-C4-C5	6.00	108.20	105.80
1	AA	373	A	N9-C4-C5	6.00	108.20	105.80
22	BA	788	A	N9-C4-C5	6.00	108.20	105.80
22	BA	1927	A	C4-C5-C6	6.00	120.00	117.00
22	BA	2411	A	C4-C5-C6	6.00	120.00	117.00
55	B8	66	A	C8-N9-C4	6.00	108.20	105.80
22	BA	155	A	C4-C5-C6	6.00	120.00	117.00
22	BA	2340	A	C4-C5-C6	6.00	120.00	117.00
22	BA	486	C	C6-N1-C2	-5.99	117.90	120.30
22	BA	1265	A	C4-C5-N7	-5.99	107.70	110.70
22	BA	1626	A	C4-C5-C6	5.99	120.00	117.00
22	BA	2757	A	C5-N7-C8	5.99	106.90	103.90
55	B8	21	A	C8-N9-C4	5.99	108.20	105.80
22	BA	2273	A	N9-C4-C5	5.99	108.20	105.80
22	BA	2430	A	O4'-C1'-N9	5.99	112.99	108.20
22	BA	1378	A	C4-C5-N7	-5.99	107.71	110.70
22	BA	2726	A	C4-C5-N7	-5.99	107.71	110.70
1	AA	1493	A	C4-C5-C6	5.99	119.99	117.00
22	BA	1937	A	C4-C5-C6	5.99	119.99	117.00
22	BA	2135	A	N9-C4-C5	5.99	108.19	105.80
27	BF	109	PRO	CA-N-CD	-5.99	103.12	111.50
22	BA	1722	A	N3-C4-N9	5.99	132.19	127.40
22	BA	2142	A	C5-C6-N1	5.99	120.69	117.70
22	BA	330	A	C5-C6-N1	5.98	120.69	117.70
1	AA	781	A	C4-C5-N7	-5.98	107.71	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1250	A	C4-C5-C6	5.98	119.99	117.00
22	BA	532	A	N3-C4-N9	5.98	132.19	127.40
22	BA	1027	A	N9-C4-C5	5.98	108.19	105.80
22	BA	1275	A	C4-C5-N7	-5.98	107.71	110.70
22	BA	2014	A	C4-C5-C6	5.98	119.99	117.00
1	AA	802	A	C4-C5-C6	5.98	119.99	117.00
22	BA	2598	A	C4-C5-N7	-5.98	107.71	110.70
23	BB	94	A	C4-C5-C6	5.98	119.99	117.00
22	BA	382	A	N9-C4-C5	5.98	108.19	105.80
22	BA	2366	A	N3-C4-N9	5.98	132.18	127.40
22	BA	2856	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1067	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1256	A	N9-C4-C5	5.98	108.19	105.80
22	BA	1009	A	C4-C5-C6	5.98	119.99	117.00
22	BA	1204	A	C5-N7-C8	5.98	106.89	103.90
22	BA	141	G	C6-C5-N7	-5.98	126.81	130.40
1	AA	630	A	N9-C4-C5	5.97	108.19	105.80
22	BA	788	A	C4-C5-N7	-5.97	107.71	110.70
22	BA	861	A	N9-C4-C5	5.97	108.19	105.80
22	BA	1549	A	C5-C6-N1	5.97	120.69	117.70
1	AA	1044	A	C4-C5-C6	5.97	119.99	117.00
22	BA	1654	A	N3-C4-N9	5.97	132.18	127.40
22	BA	1759	A	N3-C4-N9	5.97	132.18	127.40
22	BA	1987	A	N9-C4-C5	5.97	108.19	105.80
23	BB	29	A	C4-C5-C6	5.97	119.99	117.00
1	AA	523	A	C4-C5-C6	5.97	119.98	117.00
1	AA	482	A	C4-C5-C6	5.97	119.98	117.00
1	AA	1257	A	C4-C5-C6	5.97	119.98	117.00
22	BA	1373	A	N3-C4-N9	5.97	132.18	127.40
8	AH	96	MET	CA-CB-CG	5.97	123.44	113.30
22	BA	2003	A	C5-C6-N1	5.97	120.68	117.70
1	AA	327	A	N9-C4-C5	5.97	108.19	105.80
1	AA	363	A	C4-C5-N7	-5.97	107.72	110.70
1	AA	373	A	N3-C4-N9	5.97	132.17	127.40
22	BA	2392	A	C4-C5-C6	5.97	119.98	117.00
1	AA	535	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1493	A	N9-C4-C5	5.96	108.19	105.80
22	BA	586	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1363	A	N9-C4-C5	5.96	108.19	105.80
22	BA	1640	A	N3-C4-N9	5.96	132.17	127.40
22	BA	1654	A	C4-C5-C6	5.96	119.98	117.00
22	BA	2227	A	N9-C4-C5	5.96	108.18	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1035	A	N3-C4-N9	5.96	132.17	127.40
22	BA	461	C	C6-N1-C2	-5.96	117.92	120.30
22	BA	631	A	C8-N9-C4	5.96	108.18	105.80
22	BA	2792	A	N9-C4-C5	5.96	108.18	105.80
1	AA	393	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1499	A	N9-C4-C5	5.96	108.18	105.80
22	BA	794	A	N9-C4-C5	5.96	108.18	105.80
22	BA	1214	A	C4-C5-N7	-5.96	107.72	110.70
1	AA	1204	A	C4-C5-C6	5.95	119.98	117.00
1	AA	1465	A	N3-C4-N9	5.95	132.16	127.40
22	BA	71	A	N3-C4-N9	5.95	132.16	127.40
22	BA	2072	C	C6-N1-C2	-5.95	117.92	120.30
22	BA	1001	A	C4-C5-C6	5.95	119.98	117.00
55	B8	38	A	C4-C5-C6	5.95	119.97	117.00
1	AA	353	A	C4-C5-C6	5.95	119.97	117.00
22	BA	706	A	C4-C5-C6	5.95	119.97	117.00
22	BA	2757	A	N9-C4-C5	5.95	108.18	105.80
23	BB	39	A	N9-C4-C5	5.95	108.18	105.80
1	AA	129	A	C4-C5-C6	5.95	119.97	117.00
2	AB	135	LEU	CB-CG-CD2	5.95	121.11	111.00
22	BA	1641	A	C5-N7-C8	5.95	106.87	103.90
22	BA	2163	A	N9-C4-C5	5.95	108.18	105.80
1	AA	60	A	C5-N7-C8	5.95	106.87	103.90
1	AA	655	A	N3-C4-N9	5.95	132.16	127.40
22	BA	2531	A	N3-C4-N9	5.95	132.16	127.40
22	BA	2837	A	C4-C5-N7	-5.95	107.73	110.70
1	AA	28	A	N3-C4-N9	5.94	132.16	127.40
1	AA	547	A	C4-C5-C6	5.94	119.97	117.00
1	AA	792	A	N9-C4-C5	5.94	108.18	105.80
1	AA	873	A	N3-C4-N9	5.94	132.15	127.40
22	BA	5	A	N9-C4-C5	5.94	108.18	105.80
22	BA	262	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1088	A	N3-C4-N9	5.94	132.15	127.40
22	BA	1610	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1453	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1713	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1901	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1966	A	N9-C4-C5	5.94	108.17	105.80
1	AA	1105	A	C4-C5-C6	5.93	119.97	117.00
22	BA	1490	A	N9-C4-C5	5.93	108.17	105.80
22	BA	2171	A	C4-C5-C6	5.93	119.97	117.00
22	BA	83	A	C4-C5-N7	-5.93	107.73	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	599	A	N3-C4-N9	5.93	132.15	127.40
22	BA	1745	A	C4-C5-C6	5.93	119.97	117.00
22	BA	299	A	C4-C5-C6	5.93	119.97	117.00
55	B8	26	A	C4-C5-C6	5.93	119.97	117.00
1	AA	313	A	C4-C5-N7	-5.93	107.74	110.70
22	BA	64	A	N9-C4-C5	5.93	108.17	105.80
22	BA	428	A	C4-C5-C6	5.93	119.97	117.00
22	BA	1046	A	C4-C5-C6	5.93	119.97	117.00
22	BA	1387	A	N3-C4-N9	5.93	132.14	127.40
30	BI	40	CYS	CA-CB-SG	5.93	124.67	114.00
22	BA	1127	A	N9-C4-C5	5.93	108.17	105.80
22	BA	1786	A	C4-C5-C6	5.93	119.96	117.00
1	AA	1431	A	N9-C4-C5	5.93	108.17	105.80
22	BA	661	A	C5-C6-N1	5.93	120.66	117.70
22	BA	2748	A	N9-C4-C5	5.93	108.17	105.80
22	BA	2800	A	C4-C5-C6	5.93	119.96	117.00
1	AA	1396	A	C4-C5-C6	5.92	119.96	117.00
22	BA	1155	A	C4-C5-C6	5.92	119.96	117.00
22	BA	1155	A	C5-N7-C8	5.92	106.86	103.90
22	BA	2439	A	C4-C5-C6	5.92	119.96	117.00
1	AA	78	A	C4-C5-C6	5.92	119.96	117.00
22	BA	2471	A	C4-C5-C6	5.92	119.96	117.00
22	BA	2060	A	C4-C5-N7	-5.92	107.74	110.70
22	BA	1969	A	N9-C4-C5	5.92	108.17	105.80
1	AA	1151	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1362	A	C4-C5-C6	5.92	119.96	117.00
22	BA	165	A	C4-C5-N7	-5.92	107.74	110.70
22	BA	793	A	C8-N9-C4	5.92	108.17	105.80
22	BA	918	A	C4-C5-C6	5.92	119.96	117.00
22	BA	2335	A	C4-C5-N7	-5.92	107.74	110.70
1	AA	718	A	N9-C4-C5	5.92	108.17	105.80
22	BA	613	A	N9-C4-C5	5.92	108.17	105.80
1	AA	454	G	C6-C5-N7	-5.91	126.85	130.40
1	AA	753	A	C4-C5-C6	5.91	119.96	117.00
1	AA	900	A	C4-C5-C6	5.91	119.96	117.00
22	BA	217	A	C4-C5-N7	-5.91	107.74	110.70
22	BA	401	A	N3-C4-N9	5.91	132.13	127.40
22	BA	1690	A	N9-C4-C5	5.91	108.17	105.80
22	BA	1847	A	C4-C5-C6	5.91	119.96	117.00
22	BA	2020	A	C4-C5-C6	5.91	119.96	117.00
1	AA	983	A	N3-C4-N9	5.91	132.13	127.40
22	BA	415	A	C5-N7-C8	5.91	106.86	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1014	A	N9-C4-C5	5.91	108.16	105.80
22	BA	1057	A	C4-C5-C6	5.91	119.95	117.00
22	BA	207	A	C4-C5-N7	-5.91	107.75	110.70
22	BA	905	A	C4-C5-C6	5.91	119.95	117.00
22	BA	1439	A	C4-C5-C6	5.91	119.95	117.00
22	BA	2020	A	C5-N7-C8	5.91	106.85	103.90
1	AA	1513	A	C4-C5-N7	-5.91	107.75	110.70
22	BA	1477	A	N9-C4-C5	5.91	108.16	105.80
1	AA	1349	A	C4-C5-C6	5.91	119.95	117.00
1	AA	1446	A	N3-C4-N9	5.91	132.12	127.40
22	BA	64	A	N3-C4-N9	5.91	132.12	127.40
22	BA	2005	A	C4-C5-N7	-5.91	107.75	110.70
1	AA	1441	A	N9-C4-C5	5.90	108.16	105.80
22	BA	459	U	N3-C2-O2	-5.90	118.07	122.20
22	BA	256	A	N3-C4-N9	5.90	132.12	127.40
22	BA	2386	A	N9-C4-C5	5.90	108.16	105.80
22	BA	352	A	C4-C5-C6	5.90	119.95	117.00
22	BA	1431	A	C4-C5-N7	-5.90	107.75	110.70
22	BA	2037	A	N9-C4-C5	5.90	108.16	105.80
1	AA	918	A	C4-C5-C6	5.90	119.95	117.00
22	BA	2510	C	C6-N1-C2	-5.90	117.94	120.30
1	AA	532	A	N3-C4-N9	5.90	132.12	127.40
22	BA	73	A	C4-C5-C6	5.90	119.95	117.00
22	BA	925	A	C5-C6-N1	5.90	120.65	117.70
1	AA	872	A	N3-C4-N9	5.89	132.12	127.40
1	AA	974	A	C4-C5-C6	5.89	119.95	117.00
22	BA	603	A	N9-C4-C5	5.89	108.16	105.80
22	BA	1503	A	C4-C5-C6	5.89	119.95	117.00
22	BA	2471	A	C4-C5-N7	-5.89	107.75	110.70
22	BA	412	A	C4-C5-C6	5.89	119.94	117.00
1	AA	554	A	C4-C5-N7	-5.89	107.76	110.70
22	BA	1274	A	N9-C4-C5	5.89	108.16	105.80
22	BA	2662	A	N9-C4-C5	5.89	108.16	105.80
22	BA	1268	A	C4-C5-C6	5.89	119.94	117.00
22	BA	2434	A	C4-C5-N7	-5.89	107.76	110.70
22	BA	1237	A	C4-C5-C6	5.88	119.94	117.00
22	BA	2268	A	C4-C5-N7	-5.88	107.76	110.70
22	BA	2376	A	C4-C5-C6	5.88	119.94	117.00
22	BA	685	A	N9-C4-C5	5.88	108.15	105.80
22	BA	1194	A	C4-C5-C6	5.88	119.94	117.00
22	BA	675	A	C4-C5-C6	5.88	119.94	117.00
22	BA	1640	A	N9-C4-C5	5.88	108.15	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1927	A	C4-C5-N7	-5.88	107.76	110.70
22	BA	668	A	C5-N7-C8	5.88	106.84	103.90
22	BA	925	A	N3-C4-N9	5.88	132.10	127.40
22	BA	2725	A	N9-C4-C5	5.88	108.15	105.80
22	BA	750	A	C5-C6-N1	5.88	120.64	117.70
22	BA	1009	A	C5-N7-C8	5.88	106.84	103.90
22	BA	1142	A	C8-N9-C4	5.88	108.15	105.80
1	AA	996	A	C4-C5-C6	5.88	119.94	117.00
22	BA	144	A	N3-C4-N9	5.88	132.10	127.40
22	BA	204	A	C4-C5-N7	-5.88	107.76	110.70
22	BA	218	A	N3-C4-N9	5.88	132.10	127.40
22	BA	917	A	N3-C4-N9	5.88	132.10	127.40
1	AA	321	A	C4-C5-C6	5.88	119.94	117.00
22	BA	613	A	N3-C4-N9	5.88	132.10	127.40
23	BB	57	A	N3-C4-N9	5.88	132.10	127.40
1	AA	1219	A	N3-C4-N9	5.87	132.10	127.40
22	BA	802	A	C4-C5-N7	-5.87	107.76	110.70
22	BA	2530	A	C4-C5-N7	-5.87	107.76	110.70
1	AA	28	A	N9-C4-C5	5.87	108.15	105.80
1	AA	1081	A	N3-C4-N9	5.87	132.10	127.40
22	BA	2281	A	N3-C4-N9	5.87	132.10	127.40
1	AA	1394	A	C4-C5-C6	5.87	119.94	117.00
55	B8	41	A	C4-C5-C6	5.87	119.94	117.00
22	BA	1572	A	N3-C4-N9	5.87	132.09	127.40
1	AA	712	A	C5-C6-N1	5.87	120.63	117.70
1	AA	1000	A	N9-C4-C5	5.87	108.15	105.80
1	AA	746	A	N9-C4-C5	5.86	108.15	105.80
22	BA	849	A	N9-C4-C5	5.86	108.14	105.80
22	BA	909	A	C5-C6-N1	5.86	120.63	117.70
22	BA	2602	A	C8-N9-C4	5.86	108.14	105.80
22	BA	2449	U	N3-C4-C5	5.86	118.12	114.60
22	BA	2700	A	N3-C4-N9	5.86	132.09	127.40
1	AA	907	A	N9-C4-C5	5.86	108.14	105.80
22	BA	384	A	N9-C4-C5	5.86	108.14	105.80
23	BB	94	A	N3-C4-N9	5.86	132.09	127.40
1	AA	767	A	N9-C4-C5	5.86	108.14	105.80
1	AA	408	A	C4-C5-N7	-5.85	107.77	110.70
22	BA	1247	A	C4-C5-N7	-5.85	107.77	110.70
1	AA	784	A	C4-C5-C6	5.85	119.93	117.00
22	BA	2388	A	C4-C5-C6	5.85	119.93	117.00
1	AA	1081	A	N9-C4-C5	5.85	108.14	105.80
22	BA	1665	A	N3-C4-N9	5.85	132.08	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	B8	76	A	N3-C4-N9	5.85	132.08	127.40
1	AA	55	A	N9-C4-C5	5.85	108.14	105.80
1	AA	572	A	C4-C5-N7	-5.85	107.78	110.70
1	AA	663	A	N9-C4-C5	5.85	108.14	105.80
1	AA	1019	A	C4-C5-C6	5.85	119.92	117.00
1	AA	1483	A	N3-C4-N9	5.85	132.08	127.40
22	BA	877	A	C4-C5-C6	5.85	119.92	117.00
22	BA	933	A	N3-C4-N9	5.85	132.08	127.40
22	BA	1470	A	C4-C5-N7	-5.85	107.78	110.70
1	AA	1046	A	N9-C4-C5	5.84	108.14	105.80
1	AA	1080	A	C4-C5-C6	5.84	119.92	117.00
55	B8	42	A	C5-C6-N1	5.84	120.62	117.70
1	AA	72	A	C4-C5-C6	5.84	119.92	117.00
1	AA	487	A	N3-C4-N9	5.84	132.07	127.40
22	BA	1847	A	C5-N7-C8	5.84	106.82	103.90
22	BA	2119	A	C4-C5-C6	5.84	119.92	117.00
22	BA	2748	A	C5-N7-C8	5.84	106.82	103.90
1	AA	1	A	N3-C4-N9	5.84	132.07	127.40
22	BA	739	A	C4-C5-C6	5.84	119.92	117.00
22	BA	911	A	C5-N7-C8	5.84	106.82	103.90
22	BA	2173	A	N9-C4-C5	5.84	108.14	105.80
22	BA	2450	A	C4-C5-N7	-5.84	107.78	110.70
55	B8	20	U	C6-N1-C2	5.84	124.50	121.00
22	BA	990	A	C4-C5-N7	-5.84	107.78	110.70
22	BA	1819	A	N3-C4-N9	5.84	132.07	127.40
22	BA	1998	A	C5-C6-N1	5.84	120.62	117.70
22	BA	2468	A	C4-C5-C6	5.84	119.92	117.00
1	AA	179	A	C4-C5-C6	5.83	119.92	117.00
1	AA	1163	A	N9-C4-C5	5.83	108.13	105.80
55	B8	51	A	N3-C4-N9	5.83	132.07	127.40
22	BA	1535	A	N9-C4-C5	5.83	108.13	105.80
22	BA	1566	A	C8-N9-C4	5.83	108.13	105.80
55	B8	73	A	N3-C4-N9	5.83	132.07	127.40
22	BA	63	A	N3-C4-N9	5.83	132.07	127.40
22	BA	262	A	N3-C4-N9	5.83	132.07	127.40
22	BA	2461	A	N9-C4-C5	5.83	108.13	105.80
22	BA	256	A	N9-C4-C5	5.83	108.13	105.80
22	BA	2392	A	N9-C4-C5	5.83	108.13	105.80
1	AA	439	U	C5-C4-O4	-5.83	122.40	125.90
1	AA	539	A	N3-C4-N9	5.83	132.06	127.40
1	AA	1324	A	N3-C4-N9	5.83	132.06	127.40
22	BA	422	A	N3-C4-N9	5.83	132.06	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1237	A	N9-C4-C5	5.83	108.13	105.80
22	BA	751	A	N3-C4-N9	5.83	132.06	127.40
1	AA	382	A	N3-C4-N9	5.83	132.06	127.40
22	BA	1593	A	C4-C5-C6	5.83	119.91	117.00
22	BA	2088	A	N3-C4-N9	5.83	132.06	127.40
55	B8	76	A	C4-C5-C6	5.83	119.91	117.00
1	AA	865	A	N3-C4-N9	5.82	132.06	127.40
1	AA	914	A	N3-C4-N9	5.82	132.06	127.40
1	AA	1500	A	C5-N7-C8	5.82	106.81	103.90
22	BA	631	A	C4-C5-C6	5.82	119.91	117.00
22	BA	1089	A	C4-C5-C6	5.82	119.91	117.00
22	BA	1010	A	C4-C5-C6	5.82	119.91	117.00
23	BB	101	A	C4-C5-N7	-5.82	107.79	110.70
22	BA	2352	A	C4-C5-N7	-5.82	107.79	110.70
22	BA	2675	A	N3-C4-N9	5.82	132.06	127.40
1	AA	32	A	C5-C6-N1	5.82	120.61	117.70
22	BA	42	A	C4-C5-C6	5.82	119.91	117.00
22	BA	1420	A	C4-C5-N7	-5.82	107.79	110.70
22	BA	1515	A	C4-C5-C6	5.82	119.91	117.00
22	BA	1676	A	N9-C4-C5	5.82	108.13	105.80
22	BA	119	A	C4-C5-N7	-5.82	107.79	110.70
22	BA	722	A	N9-C4-C5	5.82	108.13	105.80
22	BA	1470	A	N3-C4-N9	5.82	132.05	127.40
23	BB	15	A	C4-C5-C6	5.82	119.91	117.00
1	AA	560	A	C4-C5-C6	5.82	119.91	117.00
22	BA	2740	A	N3-C4-N9	5.82	132.05	127.40
1	AA	949	A	C4-C5-N7	-5.81	107.79	110.70
22	BA	2062	A	C4-C5-C6	5.81	119.91	117.00
22	BA	2860	A	C4-C5-C6	5.81	119.91	117.00
1	AA	892	A	N3-C4-N9	5.81	132.05	127.40
22	BA	226	A	N9-C4-C5	5.81	108.12	105.80
22	BA	444	C	C6-N1-C2	-5.81	117.98	120.30
22	BA	1598	A	C4-C5-N7	-5.81	107.80	110.70
22	BA	1780	A	C4-C5-C6	5.81	119.91	117.00
22	BA	2547	A	C4-C5-C6	5.81	119.90	117.00
1	AA	461	A	N9-C4-C5	5.81	108.12	105.80
22	BA	752	A	C4-C5-C6	5.81	119.90	117.00
22	BA	849	A	N3-C4-N9	5.81	132.04	127.40
22	BA	1508	A	N9-C4-C5	5.81	108.12	105.80
22	BA	404	A	C5-N7-C8	5.81	106.80	103.90
22	BA	1970	A	C5-N7-C8	5.80	106.80	103.90
22	BA	2600	A	N3-C4-N9	5.80	132.04	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	221	A	N9-C4-C5	5.80	108.12	105.80
22	BA	362	A	N3-C4-N9	5.80	132.04	127.40
22	BA	782	A	N3-C4-N9	5.80	132.04	127.40
22	BA	449	A	C4-C5-N7	-5.80	107.80	110.70
22	BA	1274	A	N3-C4-N9	5.80	132.04	127.40
22	BA	2088	A	N9-C4-C5	5.80	108.12	105.80
1	AA	573	A	C4-C5-C6	5.80	119.90	117.00
22	BA	1515	A	C4-C5-N7	-5.80	107.80	110.70
22	BA	1785	A	N9-C4-C5	5.80	108.12	105.80
55	B8	19	G	O4'-C1'-N9	-5.80	103.56	108.20
1	AA	365	U	C5-C4-O4	5.80	129.38	125.90
22	BA	1009	A	N9-C4-C5	5.80	108.12	105.80
22	BA	1353	A	C5-C6-N1	5.80	120.60	117.70
22	BA	2101	A	C4-C5-C6	5.80	119.90	117.00
22	BA	2513	A	C4-C5-N7	-5.80	107.80	110.70
22	BA	2887	A	C4-C5-C6	5.80	119.90	117.00
22	BA	190	A	C4-C5-N7	-5.79	107.80	110.70
22	BA	1304	A	C4-C5-C6	5.79	119.90	117.00
22	BA	1912	A	C4-C5-C6	5.79	119.90	117.00
22	BA	2198	A	C8-N9-C4	5.79	108.12	105.80
1	AA	1306	A	N3-C4-N9	5.79	132.03	127.40
22	BA	1641	A	N3-C4-N9	5.79	132.03	127.40
22	BA	2328	A	N9-C4-C5	5.79	108.12	105.80
22	BA	2665	A	N3-C4-N9	5.79	132.03	127.40
1	AA	907	A	N3-C4-N9	5.79	132.03	127.40
22	BA	743	A	N9-C4-C5	5.79	108.12	105.80
22	BA	2266	A	C5-N7-C8	5.79	106.80	103.90
54	B7	8	G	C8-N9-C4	5.79	108.72	106.40
1	AA	1299	A	N9-C4-C5	5.79	108.12	105.80
22	BA	309	A	C4-C5-C6	5.79	119.89	117.00
22	BA	371	A	C4-C5-C6	5.79	119.89	117.00
22	BA	2614	A	N3-C4-N9	5.79	132.03	127.40
1	AA	1318	A	C4-C5-C6	5.79	119.89	117.00
1	AA	1500	A	N3-C4-N9	5.79	132.03	127.40
22	BA	44	A	C4-C5-N7	-5.79	107.81	110.70
22	BA	528	A	N3-C4-N9	5.79	132.03	127.40
22	BA	2435	A	N9-C4-C5	5.79	108.11	105.80
1	AA	889	A	C4-C5-N7	-5.78	107.81	110.70
22	BA	2662	A	N3-C4-N9	5.78	132.03	127.40
22	BA	2835	A	C4-C5-N7	-5.78	107.81	110.70
22	BA	2531	A	N9-C4-C5	5.78	108.11	105.80
22	BA	1676	A	N3-C4-N9	5.78	132.02	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1757	A	C8-N9-C4	5.78	108.11	105.80
22	BA	2377	A	C4-C5-C6	5.78	119.89	117.00
22	BA	2468	A	N9-C4-C5	5.78	108.11	105.80
22	BA	878	A	C4-C5-C6	5.78	119.89	117.00
22	BA	2781	A	N9-C4-C5	5.78	108.11	105.80
22	BA	592	A	C5-C6-N1	5.78	120.59	117.70
22	BA	643	A	C4-C5-C6	5.78	119.89	117.00
22	BA	1126	A	N9-C4-C5	5.78	108.11	105.80
22	BA	2031	A	C4-C5-C6	5.78	119.89	117.00
22	BA	2147	A	C4-C5-C6	5.78	119.89	117.00
22	BA	1848	A	C4-C5-N7	-5.78	107.81	110.70
1	AA	607	A	C4-C5-N7	-5.77	107.81	110.70
22	BA	1032	A	C4-C5-C6	5.77	119.89	117.00
22	BA	1392	A	C5-C6-N1	5.77	120.59	117.70
22	BA	866	A	C4-C5-C6	5.77	119.89	117.00
22	BA	959	A	N3-C4-N9	5.77	132.02	127.40
22	BA	1784	A	N3-C4-N9	5.77	132.02	127.40
29	BH	122	LEU	CA-CB-CG	5.77	128.58	115.30
22	BA	631	A	N3-C4-N9	5.77	132.02	127.40
22	BA	1787	A	C5-C6-N1	5.77	120.58	117.70
1	AA	554	A	C4-C5-C6	5.77	119.88	117.00
22	BA	111	A	C4-C5-C6	5.77	119.88	117.00
22	BA	1272	A	C4-C5-N7	-5.77	107.82	110.70
22	BA	2031	A	N3-C4-N9	5.77	132.01	127.40
22	BA	2433	A	N3-C4-N9	5.77	132.01	127.40
1	AA	1158	C	N1-C2-O2	5.77	122.36	118.90
1	AA	389	A	C5-C6-N1	5.76	120.58	117.70
22	BA	1073	A	N9-C4-C5	5.76	108.11	105.80
22	BA	53	A	N9-C4-C5	5.76	108.11	105.80
22	BA	751	A	N9-C4-C5	5.76	108.11	105.80
53	B5	24	PRO	CA-N-CD	-5.76	103.43	111.50
1	AA	389	A	N3-C4-N9	5.76	132.01	127.40
22	BA	226	A	N3-C4-N9	5.76	132.01	127.40
22	BA	1029	A	N3-C4-N9	5.76	132.01	127.40
22	BA	1603	A	C5-C6-N1	5.76	120.58	117.70
1	AA	696	A	N3-C4-N9	5.76	132.00	127.40
22	BA	1073	A	N3-C4-N9	5.76	132.00	127.40
22	BA	2461	A	C5-C6-N1	5.76	120.58	117.70
22	BA	2518	A	C5-C6-N1	5.76	120.58	117.70
1	AA	495	A	C4-C5-C6	5.75	119.88	117.00
22	BA	643	A	C8-N9-C4	5.75	108.10	105.80
1	AA	129	A	C4-C5-N7	-5.75	107.82	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	321	A	C4-C5-N7	-5.75	107.82	110.70
1	AA	1503	A	N9-C4-C5	5.75	108.10	105.80
22	BA	582	A	N9-C4-C5	5.75	108.10	105.80
22	BA	1596	A	C4-C5-C6	5.75	119.88	117.00
22	BA	2635	A	C5-C6-N1	5.75	120.58	117.70
1	AA	1447	A	C5-C6-N1	5.75	120.58	117.70
22	BA	727	A	N9-C4-C5	5.75	108.10	105.80
22	BA	945	A	C4-C5-C6	5.75	119.88	117.00
23	BB	75	G	C5-C6-N1	5.75	114.38	111.50
1	AA	1394	A	N9-C4-C5	5.75	108.10	105.80
1	AA	44	A	C4-C5-N7	-5.75	107.83	110.70
22	BA	911	A	N3-C4-N9	5.75	132.00	127.40
1	AA	673	A	C4-C5-N7	-5.75	107.83	110.70
1	AA	1117	A	C4-C5-C6	5.75	119.87	117.00
22	BA	670	A	C4-C5-C6	5.75	119.87	117.00
22	BA	743	A	N3-C4-N9	5.75	132.00	127.40
1	AA	1239	A	N9-C4-C5	5.75	108.10	105.80
22	BA	111	A	C4-C5-N7	-5.75	107.83	110.70
22	BA	439	A	C5-C6-N1	5.75	120.57	117.70
22	BA	1001	A	C4-C5-N7	-5.75	107.83	110.70
22	BA	1586	A	C4-C5-N7	-5.75	107.83	110.70
22	BA	1932	A	C4-C5-C6	5.75	119.87	117.00
22	BA	2835	A	C4-C5-C6	5.74	119.87	117.00
1	AA	282	A	C4-C5-C6	5.74	119.87	117.00
22	BA	1028	A	C5-C6-N1	5.74	120.57	117.70
1	AA	236	A	C4-C5-C6	5.74	119.87	117.00
1	AA	365	U	C2-N3-C4	5.74	130.44	127.00
22	BA	1100	C	C6-N1-C2	-5.74	118.00	120.30
22	BA	1194	A	C4-C5-N7	-5.74	107.83	110.70
22	BA	2381	A	C4-C5-C6	5.74	119.87	117.00
1	AA	596	A	C5-C6-N1	5.74	120.57	117.70
22	BA	1088	A	N9-C4-C5	5.74	108.09	105.80
22	BA	1918	A	N3-C4-N9	5.74	131.99	127.40
1	AA	814	A	N3-C4-N9	5.74	131.99	127.40
22	BA	460	A	N3-C4-N9	5.74	131.99	127.40
22	BA	2080	A	C5-C6-N1	5.74	120.57	117.70
22	BA	2015	A	N3-C4-N9	5.74	131.99	127.40
1	AA	1016	A	C4-C5-N7	-5.73	107.83	110.70
22	BA	756	A	N3-C4-N9	5.73	131.99	127.40
22	BA	2873	A	C4-C5-N7	-5.73	107.83	110.70
1	AA	746	A	C5-C6-N1	5.73	120.57	117.70
22	BA	621	A	C4-C5-N7	-5.73	107.83	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	199	A	N3-C4-N9	5.73	131.98	127.40
1	AA	243	A	C4-C5-C6	5.73	119.86	117.00
1	AA	918	A	C4-C5-N7	-5.73	107.83	110.70
22	BA	927	A	C4-C5-N7	-5.73	107.84	110.70
22	BA	979	A	C4-C5-N7	-5.73	107.83	110.70
22	BA	1591	A	N3-C4-N9	5.73	131.98	127.40
22	BA	2425	A	N3-C4-N9	5.73	131.98	127.40
22	BA	2705	A	N3-C4-N9	5.73	131.98	127.40
1	AA	1055	A	N3-C4-N9	5.73	131.98	127.40
1	AA	1299	A	C4-C5-N7	-5.73	107.84	110.70
22	BA	1070	A	C4-C5-C6	5.73	119.86	117.00
22	BA	2434	A	C4-C5-C6	5.73	119.86	117.00
1	AA	608	A	N3-C4-N9	5.73	131.98	127.40
1	AA	1261	A	N3-C4-N9	5.73	131.98	127.40
22	BA	1302	A	N3-C4-N9	5.73	131.98	127.40
22	BA	1772	A	C4-C5-N7	-5.73	107.84	110.70
55	B8	6	A	N3-C4-N9	5.73	131.98	127.40
1	AA	33	A	N3-C4-N9	5.72	131.98	127.40
22	BA	1144	A	N3-C4-N9	5.72	131.98	127.40
22	BA	2020	A	N3-C4-N9	5.72	131.98	127.40
22	BA	2469	A	C5-N7-C8	5.72	106.76	103.90
22	BA	2598	A	C4-C5-C6	5.72	119.86	117.00
1	AA	470	C	N1-C2-O2	5.72	122.33	118.90
1	AA	1180	A	C4-C5-N7	-5.72	107.84	110.70
1	AA	1246	A	C4-C5-N7	-5.72	107.84	110.70
22	BA	825	A	C4-C5-C6	5.72	119.86	117.00
1	AA	119	A	C4-C5-C6	5.72	119.86	117.00
22	BA	262	A	C4-C5-N7	-5.72	107.84	110.70
22	BA	556	A	N3-C4-N9	5.72	131.98	127.40
22	BA	1794	A	N3-C4-N9	5.72	131.98	127.40
22	BA	2199	A	N3-C4-N9	5.72	131.97	127.40
23	BB	24	G	C6-N1-C2	-5.72	121.67	125.10
23	BB	46	A	C4-C5-N7	-5.72	107.84	110.70
1	AA	913	A	C4-C5-C6	5.72	119.86	117.00
22	BA	668	A	C8-N9-C4	5.72	108.09	105.80
1	AA	676	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1428	A	C4-C5-N7	-5.72	107.84	110.70
22	BA	1156	A	N9-C4-C5	5.72	108.09	105.80
22	BA	1566	A	N9-C4-C5	5.72	108.09	105.80
22	BA	1609	A	N3-C4-N9	5.72	131.97	127.40
22	BA	2051	A	N3-C4-N9	5.72	131.97	127.40
1	AA	374	A	C4-C5-N7	-5.71	107.84	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1329	A	C4-C5-C6	5.71	119.86	117.00
2	AB	212	LEU	CA-CB-CG	5.71	128.44	115.30
22	BA	666	A	N3-C4-N9	5.71	131.97	127.40
22	BA	2227	A	C4-C5-N7	-5.71	107.84	110.70
22	BA	2447	G	C5-C6-N1	5.71	114.36	111.50
1	AA	819	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	1377	A	C4-C5-C6	5.71	119.86	117.00
22	BA	19	A	N3-C4-N9	5.71	131.97	127.40
22	BA	661	A	N3-C4-N9	5.71	131.97	127.40
22	BA	1808	A	C4-C5-C6	5.71	119.85	117.00
22	BA	2274	A	C4-C5-N7	-5.71	107.85	110.70
1	AA	288	A	N3-C4-N9	5.71	131.97	127.40
1	AA	498	A	C6-N1-C2	-5.71	115.18	118.60
22	BA	53	A	C4-C5-C6	5.71	119.85	117.00
22	BA	71	A	C8-N9-C4	5.71	108.08	105.80
22	BA	608	A	C5-C6-N1	5.71	120.55	117.70
22	BA	721	A	N3-C4-N9	5.70	131.96	127.40
22	BA	2657	A	C4-C5-C6	5.70	119.85	117.00
1	AA	825	A	C4-C5-C6	5.70	119.85	117.00
22	BA	892	A	N9-C4-C5	5.70	108.08	105.80
54	B7	8	G	OP1-P-OP2	5.70	128.15	119.60
55	B8	58	A	N3-C4-N9	5.70	131.96	127.40
1	AA	994	A	N3-C4-N9	5.70	131.96	127.40
22	BA	1030	C	C6-N1-C2	-5.70	118.02	120.30
1	AA	253	A	N9-C4-C5	5.70	108.08	105.80
22	BA	609	A	C4-C5-C6	5.70	119.85	117.00
1	AA	116	A	C5-C6-N1	5.70	120.55	117.70
1	AA	171	A	C4-C5-C6	5.70	119.85	117.00
22	BA	1142	A	C4-C5-C6	5.70	119.85	117.00
22	BA	2882	A	C4-C5-C6	5.70	119.85	117.00
1	AA	532	A	N9-C4-C5	5.70	108.08	105.80
1	AA	1500	A	C4-C5-C6	5.70	119.85	117.00
22	BA	575	A	C5-N7-C8	5.70	106.75	103.90
22	BA	2469	A	N3-C4-N9	5.69	131.96	127.40
1	AA	431	A	C4-C5-C6	5.69	119.85	117.00
22	BA	685	A	N3-C4-N9	5.69	131.95	127.40
22	BA	1504	A	C4-C5-C6	5.69	119.85	117.00
22	BA	2094	A	C5-C6-N1	5.69	120.55	117.70
22	BA	2154	A	N3-C4-N9	5.69	131.95	127.40
1	AA	162	A	N9-C4-C5	5.69	108.08	105.80
22	BA	947	A	N9-C4-C5	5.69	108.08	105.80
22	BA	199	A	C4-C5-C6	5.69	119.84	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	382	A	N3-C4-N9	5.69	131.95	127.40
22	BA	1801	A	N9-C4-C5	5.69	108.07	105.80
22	BA	255	A	N9-C4-C5	5.68	108.07	105.80
22	BA	693	A	N9-C4-C5	5.68	108.07	105.80
22	BA	1134	A	N3-C4-N9	5.68	131.95	127.40
22	BA	1829	A	N3-C4-N9	5.68	131.95	127.40
1	AA	819	A	C4-C5-C6	5.68	119.84	117.00
22	BA	1353	A	C4-C5-C6	5.68	119.84	117.00
22	BA	2501	C	C6-N1-C1'	5.68	127.62	120.80
1	AA	313	A	C5-C6-N1	5.68	120.54	117.70
22	BA	2033	A	C4-C5-C6	5.68	119.84	117.00
22	BA	2198	A	N9-C4-C5	5.68	108.07	105.80
22	BA	2335	A	N3-C4-N9	5.68	131.94	127.40
22	BA	896	A	N9-C4-C5	5.68	108.07	105.80
1	AA	465	A	N3-C4-N9	5.68	131.94	127.40
1	AA	919	A	C4-C5-N7	-5.68	107.86	110.70
1	AA	1055	A	N9-C4-C5	5.68	108.07	105.80
22	BA	845	A	C5-C6-N1	5.68	120.54	117.70
22	BA	1678	A	C4-C5-N7	-5.68	107.86	110.70
22	BA	1754	A	N3-C4-N9	5.68	131.94	127.40
22	BA	1913	A	C8-N9-C4	5.68	108.07	105.80
22	BA	223	A	C8-N9-C4	5.67	108.07	105.80
22	BA	2820	A	C4-C5-C6	5.67	119.84	117.00
22	BA	2821	A	N9-C4-C5	5.67	108.07	105.80
22	BA	2837	A	C5-C6-N1	5.67	120.54	117.70
22	BA	2750	A	C4-C5-C6	5.67	119.84	117.00
22	BA	2031	A	N9-C4-C5	5.67	108.07	105.80
22	BA	1354	A	N3-C4-N9	5.67	131.94	127.40
1	AA	906	A	C4-C5-N7	-5.67	107.87	110.70
1	AA	1465	A	N9-C4-C5	5.67	108.07	105.80
22	BA	1253	A	C5-C6-N1	5.67	120.53	117.70
22	BA	118	A	N9-C4-C5	5.67	108.07	105.80
22	BA	1672	A	N3-C4-N9	5.67	131.93	127.40
22	BA	1700	A	N3-C4-N9	5.67	131.93	127.40
22	BA	2241	A	N3-C4-N9	5.67	131.93	127.40
22	BA	2327	A	N3-C4-N9	5.67	131.93	127.40
23	BB	94	A	N9-C4-C5	5.67	108.07	105.80
1	AA	1151	A	C5-C6-N1	5.67	120.53	117.70
22	BA	2872	A	C6-N1-C2	5.67	122.00	118.60
22	BA	928	A	N3-C4-N9	5.66	131.93	127.40
22	BA	1086	A	C4-C5-C6	5.66	119.83	117.00
22	BA	2114	A	N9-C4-C5	5.66	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	621	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	1913	A	N9-C4-C5	5.66	108.06	105.80
22	BA	910	A	C8-N9-C4	5.66	108.06	105.80
22	BA	1821	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	2014	A	C4-C5-N7	-5.66	107.87	110.70
1	AA	160	A	C4-C5-C6	5.65	119.83	117.00
1	AA	329	A	N3-C4-N9	5.65	131.92	127.40
1	AA	715	A	N3-C4-N9	5.65	131.92	127.40
22	BA	1936	A	C5-C6-N1	5.65	120.53	117.70
1	AA	44	A	C4-C5-C6	5.65	119.83	117.00
1	AA	151	A	C4-C5-N7	-5.65	107.87	110.70
1	AA	767	A	N3-C4-N9	5.65	131.92	127.40
1	AA	959	A	C4-C5-N7	-5.65	107.87	110.70
1	AA	1374	A	N3-C4-N9	5.65	131.92	127.40
22	BA	1020	A	C4-C5-C6	5.65	119.83	117.00
22	BA	1548	A	N9-C4-C5	5.65	108.06	105.80
22	BA	2003	A	N3-C4-N9	5.65	131.92	127.40
1	AA	196	A	C4-C5-C6	5.65	119.83	117.00
22	BA	282	A	N9-C4-C5	5.65	108.06	105.80
22	BA	439	A	N3-C4-N9	5.65	131.92	127.40
22	BA	1977	A	N3-C4-N9	5.65	131.92	127.40
1	AA	459	A	C5-C6-N1	5.65	120.52	117.70
22	BA	2142	A	N9-C4-C5	5.65	108.06	105.80
1	AA	676	A	C4-C5-N7	-5.65	107.88	110.70
22	BA	1670	C	N1-C2-O2	5.65	122.29	118.90
22	BA	1803	A	C4-C5-C6	5.65	119.82	117.00
22	BA	2585	U	O4'-C1'-N1	5.64	112.72	108.20
1	AA	1289	A	C4-C5-C6	5.64	119.82	117.00
22	BA	1321	A	N9-C4-C5	5.64	108.06	105.80
22	BA	2433	A	C8-N9-C4	5.64	108.06	105.80
22	BA	2635	A	N9-C4-C5	5.64	108.06	105.80
1	AA	792	A	C5-C6-N1	5.64	120.52	117.70
22	BA	1802	A	N3-C4-N9	5.64	131.91	127.40
22	BA	2761	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	1299	A	C8-N9-C4	5.64	108.06	105.80
22	BA	1504	A	C4-C5-N7	-5.64	107.88	110.70
22	BA	2893	A	N9-C4-C5	5.64	108.06	105.80
1	AA	415	A	N3-C4-N9	5.64	131.91	127.40
1	AA	1311	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	448	A	N3-C4-N9	5.63	131.91	127.40
1	AA	456	A	C4-C5-C6	5.63	119.82	117.00
1	AA	489	C	O4'-C1'-N1	5.63	112.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1151	A	C5-C6-N1	5.63	120.52	117.70
22	BA	2513	A	N3-C4-N9	5.63	131.91	127.40
22	BA	2837	A	C4-C5-C6	5.63	119.82	117.00
55	B8	42	A	C4-C5-C6	5.63	119.82	117.00
22	BA	693	A	C5-C6-N1	5.63	120.52	117.70
23	BB	78	A	C4-C5-C6	5.63	119.82	117.00
22	BA	126	A	C8-N9-C4	5.63	108.05	105.80
22	BA	160	A	C4-C5-C6	5.63	119.81	117.00
22	BA	432	A	C4-C5-C6	5.63	119.81	117.00
22	BA	673	C	N1-C2-N3	5.63	123.14	119.20
22	BA	984	A	N3-C4-N9	5.63	131.91	127.40
22	BA	1490	A	N3-C4-N9	5.63	131.91	127.40
22	BA	1632	A	C4-C5-N7	-5.63	107.89	110.70
22	BA	1650	A	C5-C6-N1	5.63	120.52	117.70
22	BA	1783	A	N9-C4-C5	5.63	108.05	105.80
22	BA	152	A	N3-C4-N9	5.63	131.90	127.40
22	BA	501	A	C4-C5-C6	5.63	119.81	117.00
1	AA	696	A	C5-N7-C8	5.63	106.72	103.90
1	AA	919	A	C4-C5-C6	5.63	119.81	117.00
22	BA	721	A	N9-C4-C5	5.63	108.05	105.80
22	BA	1571	A	N9-C4-C5	5.63	108.05	105.80
22	BA	1583	A	C4-C5-C6	5.63	119.81	117.00
1	AA	900	A	C4-C5-N7	-5.63	107.89	110.70
22	BA	761	A	C4-C5-N7	-5.63	107.89	110.70
1	AA	728	A	N3-C4-N9	5.62	131.90	127.40
22	BA	1111	A	N3-C4-N9	5.62	131.90	127.40
1	AA	872	A	C5-C6-N1	5.62	120.51	117.70
22	BA	466	A	C4-C5-N7	-5.62	107.89	110.70
22	BA	1147	A	C4-C5-C6	5.62	119.81	117.00
55	B8	51	A	C4-C5-C6	5.62	119.81	117.00
1	AA	411	A	C4-C5-C6	5.62	119.81	117.00
1	AA	499	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	502	A	C5-C6-N1	5.62	120.51	117.70
1	AA	787	A	C4-C5-C6	5.62	119.81	117.00
19	AS	3	ARG	N-CA-C	-5.62	95.82	111.00
22	BA	191	A	N3-C4-N9	5.62	131.90	127.40
22	BA	270	A	C4-C5-N7	-5.62	107.89	110.70
22	BA	300	A	C4-C5-C6	5.62	119.81	117.00
22	BA	1111	A	N9-C4-C5	5.62	108.05	105.80
1	AA	1499	A	C4-C5-C6	5.62	119.81	117.00
22	BA	2015	A	N9-C4-C5	5.62	108.05	105.80
1	AA	510	A	C4-C5-C6	5.62	119.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	815	A	C4-C5-C6	5.62	119.81	117.00
22	BA	2366	A	N9-C4-C5	5.62	108.05	105.80
22	BA	197	A	N9-C4-C5	5.62	108.05	105.80
22	BA	213	A	C4-C5-C6	5.62	119.81	117.00
22	BA	1810	A	N9-C4-C5	5.62	108.05	105.80
22	BA	2590	A	N3-C4-N9	5.62	131.89	127.40
1	AA	958	A	C4-C5-C6	5.61	119.81	117.00
22	BA	2037	A	C4-C5-C6	5.61	119.81	117.00
1	AA	439	U	C2-N3-C4	-5.61	123.63	127.00
1	AA	496	A	N3-C4-N9	5.61	131.89	127.40
1	AA	784	A	C4-C5-N7	-5.61	107.89	110.70
22	BA	627	A	C4-C5-N7	-5.61	107.89	110.70
22	BA	2019	A	C4-C5-N7	-5.61	107.89	110.70
22	BA	2764	A	C4-C5-C6	5.61	119.81	117.00
1	AA	509	A	N3-C4-N9	5.61	131.89	127.40
22	BA	2117	A	C4-C5-C6	5.61	119.81	117.00
1	AA	77	A	N9-C4-C5	5.61	108.04	105.80
1	AA	327	A	N3-C4-N9	5.61	131.88	127.40
1	AA	753	A	C4-C5-N7	-5.61	107.90	110.70
22	BA	1876	A	N9-C4-C5	5.61	108.04	105.80
22	BA	2572	A	N9-C4-C5	5.61	108.04	105.80
1	AA	8	A	C8-N9-C4	5.61	108.04	105.80
22	BA	2590	A	C4-C5-C6	5.61	119.80	117.00
1	AA	1285	A	C4-C5-C6	5.60	119.80	117.00
22	BA	1359	A	N9-C4-C5	5.60	108.04	105.80
22	BA	1632	A	C5-C6-N1	5.60	120.50	117.70
22	BA	2278	A	N3-C4-N9	5.60	131.88	127.40
22	BA	104	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	233	A	N3-C4-N9	5.60	131.88	127.40
22	BA	1772	A	C4-C5-C6	5.60	119.80	117.00
22	BA	251	A	N9-C4-C5	5.60	108.04	105.80
22	BA	2459	A	N9-C4-C5	5.60	108.04	105.80
1	AA	766	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	541	A	C5-C6-N1	5.60	120.50	117.70
22	BA	1336	A	C5-C6-N1	5.60	120.50	117.70
1	AA	365	U	N1-C2-O2	5.60	126.72	122.80
1	AA	414	A	C4-C5-C6	5.60	119.80	117.00
1	AA	935	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	1157	A	N3-C4-N9	5.60	131.88	127.40
22	BA	278	A	N9-C4-C5	5.60	108.04	105.80
22	BA	1393	A	N9-C4-C5	5.60	108.04	105.80
22	BA	764	A	C4-C5-N7	-5.60	107.90	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2346	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	892	A	N3-C4-N9	5.59	131.88	127.40
22	BA	173	A	N3-C4-N9	5.59	131.87	127.40
22	BA	1028	A	N9-C4-C5	5.59	108.04	105.80
22	BA	1854	A	N9-C4-C5	5.59	108.04	105.80
1	AA	270	A	N3-C4-N9	5.59	131.87	127.40
22	BA	2189	U	P-O3'-C3'	5.59	126.41	119.70
22	BA	2810	A	C4-C5-N7	-5.59	107.90	110.70
22	BA	71	A	C4-C5-C6	5.59	119.79	117.00
22	BA	943	A	N3-C4-N9	5.59	131.87	127.40
22	BA	988	A	C4-C5-C6	5.59	119.79	117.00
22	BA	2052	A	C5-C6-N1	5.59	120.49	117.70
55	B8	69	A	C5-C6-N1	5.59	120.49	117.70
1	AA	1357	A	C5-N7-C8	5.58	106.69	103.90
22	BA	917	A	N9-C4-C5	5.58	108.03	105.80
22	BA	2706	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	142	A	N3-C4-N9	5.58	131.87	127.40
22	BA	1378	A	C4-C5-C6	5.58	119.79	117.00
1	AA	1333	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	38	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	207	A	C4-C5-C6	5.58	119.79	117.00
22	BA	1269	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	1302	A	N9-C4-C5	5.58	108.03	105.80
22	BA	2284	A	N9-C4-C5	5.58	108.03	105.80
22	BA	2856	A	N3-C4-N9	5.58	131.86	127.40
22	BA	2094	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	1853	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	131	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	663	A	N3-C4-N9	5.57	131.86	127.40
1	AA	964	A	N3-C4-N9	5.57	131.86	127.40
22	BA	501	A	C5-N7-C8	5.57	106.69	103.90
1	AA	452	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	787	A	C8-N9-C4	5.57	108.03	105.80
1	AA	431	A	C6-N1-C2	5.57	121.94	118.60
1	AA	622	A	C5-C6-N1	5.57	120.48	117.70
22	BA	213	A	N3-C4-N9	5.57	131.85	127.40
22	BA	742	A	N3-C4-N9	5.57	131.85	127.40
22	BA	749	A	C4-C5-N7	-5.57	107.92	110.70
22	BA	1548	A	N3-C4-N9	5.57	131.85	127.40
1	AA	197	A	C4-C5-C6	5.57	119.78	117.00
1	AA	371	A	C4-C5-C6	5.57	119.78	117.00
1	AA	792	A	C8-N9-C4	5.57	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1366	A	C4-C5-N7	-5.57	107.92	110.70
22	BA	2792	A	N3-C4-N9	5.57	131.85	127.40
1	AA	794	A	N9-C4-C5	5.56	108.03	105.80
1	AA	1350	A	N3-C4-N9	5.56	131.85	127.40
22	BA	459	U	N1-C2-O2	5.56	126.69	122.80
22	BA	1632	A	C4-C5-C6	5.56	119.78	117.00
22	BA	2411	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	1398	A	C4-C5-N7	-5.56	107.92	110.70
22	BA	1689	A	N3-C4-N9	5.56	131.85	127.40
22	BA	1815	A	N9-C4-C5	5.56	108.02	105.80
22	BA	2721	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	300	A	N9-C4-C5	5.56	108.02	105.80
1	AA	768	A	C4-C5-N7	-5.56	107.92	110.70
22	BA	715	A	N9-C4-C5	5.56	108.02	105.80
22	BA	2090	A	N9-C4-C5	5.56	108.02	105.80
22	BA	2711	A	C4-C5-N7	-5.56	107.92	110.70
22	BA	2821	A	N3-C4-N9	5.56	131.85	127.40
22	BA	156	A	N3-C4-N9	5.56	131.85	127.40
22	BA	299	A	N9-C4-C5	5.56	108.02	105.80
22	BA	1214	A	C4-C5-C6	5.56	119.78	117.00
22	BA	1744	A	N3-C4-N9	5.56	131.85	127.40
1	AA	1429	A	N3-C4-N9	5.55	131.84	127.40
22	BA	176	A	N9-C4-C5	5.55	108.02	105.80
22	BA	502	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	526	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	1548	A	C5-C6-N1	5.55	120.48	117.70
1	AA	1191	A	C5-N7-C8	5.55	106.68	103.90
1	AA	1012	A	C5-C6-N1	5.55	120.48	117.70
22	BA	480	A	N3-C4-N9	5.55	131.84	127.40
22	BA	1652	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	792	A	C8-N9-C4	5.55	108.02	105.80
22	BA	1304	A	N9-C4-C5	5.55	108.02	105.80
22	BA	2809	A	N9-C4-C5	5.55	108.02	105.80
22	BA	2469	A	N9-C4-C5	5.54	108.02	105.80
1	AA	274	A	N3-C4-N9	5.54	131.84	127.40
1	AA	1197	A	N9-C4-C5	5.54	108.02	105.80
22	BA	1789	A	N9-C4-C5	5.54	108.02	105.80
22	BA	1791	A	C4-C5-C6	5.54	119.77	117.00
22	BA	1932	A	C5-C6-N1	5.54	120.47	117.70
22	BA	2070	A	C4-C5-C6	5.54	119.77	117.00
22	BA	2082	A	N3-C4-N9	5.54	131.83	127.40
22	BA	722	A	N3-C4-N9	5.54	131.83	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	734	A	C4-C5-N7	-5.54	107.93	110.70
22	BA	1054	A	N3-C4-N9	5.54	131.83	127.40
22	BA	2013	A	N9-C4-C5	5.54	108.02	105.80
1	AA	1375	A	N3-C4-N9	5.54	131.83	127.40
1	AA	553	A	C4-C5-N7	-5.54	107.93	110.70
22	BA	391	A	C8-N9-C4	5.54	108.02	105.80
1	AA	439	U	C2-N1-C1'	5.54	124.34	117.70
1	AA	1000	A	N3-C4-N9	5.53	131.83	127.40
22	BA	348	A	N3-C4-N9	5.53	131.83	127.40
22	BA	563	A	N3-C4-N9	5.53	131.83	127.40
22	BA	644	A	C4-C5-N7	-5.53	107.93	110.70
22	BA	910	A	C4-C5-C6	5.53	119.77	117.00
22	BA	1327	A	C4-C5-N7	-5.53	107.93	110.70
55	B8	6	A	C5-C6-N1	5.53	120.47	117.70
22	BA	1387	A	N9-C4-C5	5.53	108.01	105.80
1	AA	55	A	C4-C5-N7	-5.53	107.94	110.70
17	AQ	16	LYS	N-CA-CB	-5.53	100.64	110.60
22	BA	2099	U	C5'-C4'-O4'	5.53	115.74	109.10
22	BA	1622	G	N9-C4-C5	-5.53	103.19	105.40
22	BA	2388	A	C4-C5-N7	-5.53	107.94	110.70
23	BB	53	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	460	A	N3-C4-N9	5.53	131.82	127.40
22	BA	1275	A	C4-C5-C6	5.53	119.76	117.00
22	BA	1952	A	N3-C4-N9	5.53	131.82	127.40
22	BA	2900	A	N3-C4-N9	5.53	131.82	127.40
22	BA	748	G	O4'-C1'-N9	5.53	112.62	108.20
22	BA	1129	A	C4-C5-C6	5.53	119.76	117.00
22	BA	1749	A	C4-C5-N7	-5.53	107.94	110.70
22	BA	2119	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	1531	A	N3-C4-N9	5.52	131.82	127.40
22	BA	616	A	N9-C4-C5	5.52	108.01	105.80
1	AA	754	C	C2-N1-C1'	5.52	124.88	118.80
22	BA	1262	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	1544	A	N3-C4-N9	5.52	131.82	127.40
1	AA	663	A	C5-C6-N1	5.52	120.46	117.70
22	BA	152	A	N9-C4-C5	5.52	108.01	105.80
22	BA	1672	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	2700	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	187	G	N1-C6-O6	-5.52	116.59	119.90
22	BA	1477	A	N3-C4-N9	5.52	131.81	127.40
22	BA	1698	A	C4-C5-C6	5.52	119.76	117.00
22	BA	1757	A	N3-C4-N9	5.52	131.81	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1022	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	1495	U	C2-N1-C1'	5.52	124.32	117.70
22	BA	265	A	C4-C5-C6	5.52	119.76	117.00
22	BA	1260	A	N3-C4-N9	5.52	131.81	127.40
22	BA	1260	A	C4-C5-N7	-5.51	107.94	110.70
22	BA	2837	A	N3-C4-N9	5.51	131.81	127.40
22	BA	2850	A	N3-C4-N9	5.51	131.81	127.40
1	AA	1188	A	C4-C5-N7	-5.51	107.94	110.70
22	BA	1431	A	N3-C4-N9	5.51	131.81	127.40
22	BA	1544	A	C4-C5-N7	-5.51	107.94	110.70
22	BA	2799	A	C5-C6-N1	5.51	120.46	117.70
55	B8	58	A	C5-C6-N1	5.51	120.46	117.70
1	AA	777	A	C4-C5-N7	-5.51	107.95	110.70
22	BA	654	A	N3-C4-N9	5.51	131.81	127.40
22	BA	764	A	C5-N7-C8	5.51	106.65	103.90
22	BA	1496	A	C4-C5-C6	5.51	119.75	117.00
1	AA	1287	A	C4-C5-N7	-5.51	107.95	110.70
2	AB	205	ASP	OD1-CG-OD2	-5.51	112.84	123.30
22	BA	504	A	N9-C4-C5	5.50	108.00	105.80
22	BA	1626	A	N3-C4-N9	5.50	131.80	127.40
1	AA	74	A	C4-C5-C6	5.50	119.75	117.00
1	AA	493	A	C4-C5-C6	5.50	119.75	117.00
1	AA	1346	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	503	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	789	A	C4-C5-C6	5.50	119.75	117.00
22	BA	1175	A	N3-C4-N9	5.50	131.80	127.40
22	BA	2042	A	N3-C4-N9	5.50	131.80	127.40
22	BA	2886	A	N3-C4-N9	5.50	131.80	127.40
23	BB	99	A	N3-C4-N9	5.50	131.80	127.40
1	AA	195	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	1759	A	C4-C5-C6	5.50	119.75	117.00
22	BA	2776	A	C4-C5-C6	5.50	119.75	117.00
22	BA	2813	A	N9-C4-C5	5.50	108.00	105.80
55	B8	69	A	C4-C5-C6	5.50	119.75	117.00
22	BA	160	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	1396	A	N3-C4-N9	5.50	131.80	127.40
22	BA	299	A	N3-C4-N9	5.50	131.80	127.40
22	BA	1155	A	N9-C4-C5	5.50	108.00	105.80
22	BA	2358	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	2873	A	C4-C5-C6	5.50	119.75	117.00
1	AA	238	A	C4-C5-C6	5.50	119.75	117.00
1	AA	1360	A	C4-C5-N7	-5.50	107.95	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	172	A	N3-C4-N9	5.50	131.80	127.40
22	BA	1365	A	N3-C4-N9	5.50	131.80	127.40
22	BA	1545	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	1773	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	2758	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	1130	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	223	A	C4-C5-C6	5.50	119.75	117.00
22	BA	661	A	C4-C5-C6	5.50	119.75	117.00
22	BA	1885	A	C4-C5-C6	5.50	119.75	117.00
22	BA	2309	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	911	A	N9-C4-C5	5.49	108.00	105.80
1	AA	77	A	C5-C6-N1	5.49	120.44	117.70
22	BA	199	A	C4-C5-N7	-5.49	107.95	110.70
22	BA	1809	A	C4-C5-C6	5.49	119.75	117.00
22	BA	2314	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	790	A	N3-C4-N9	5.49	131.79	127.40
22	BA	56	A	N3-C4-N9	5.49	131.79	127.40
22	BA	1677	A	N3-C4-N9	5.49	131.79	127.40
22	BA	2227	A	N3-C4-N9	5.49	131.79	127.40
55	B8	14	A	N9-C4-C5	5.49	108.00	105.80
22	BA	2736	A	C4-C5-C6	5.49	119.74	117.00
22	BA	125	A	C4-C5-C6	5.49	119.74	117.00
22	BA	2352	A	N3-C4-N9	5.49	131.79	127.40
1	AA	1179	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	1396	A	N9-C4-C5	5.48	107.99	105.80
1	AA	59	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	146	A	N3-C4-N9	5.48	131.78	127.40
22	BA	294	A	C8-N9-C4	5.48	107.99	105.80
22	BA	1739	A	C5-N7-C8	5.48	106.64	103.90
22	BA	2068	U	N1-C2-O2	5.48	126.64	122.80
22	BA	2626	C	C6-N1-C2	-5.48	118.11	120.30
1	AA	478	A	N3-C4-N9	5.48	131.78	127.40
22	BA	84	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	984	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	167	A	N3-C4-N9	5.48	131.78	127.40
1	AA	78	A	N3-C4-N9	5.48	131.78	127.40
1	AA	336	A	C5-C6-N1	5.48	120.44	117.70
1	AA	696	A	N9-C4-C5	5.48	107.99	105.80
22	BA	959	A	C4-C5-C6	5.48	119.74	117.00
22	BA	1593	A	C5-C6-N1	5.47	120.44	117.70
22	BA	2298	A	C4-C5-N7	-5.47	107.96	110.70
22	BA	94	A	N3-C4-N9	5.47	131.78	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	602	A	C4-C5-C6	5.47	119.74	117.00
22	BA	2392	A	N3-C4-N9	5.47	131.78	127.40
1	AA	655	A	C5-C6-N1	5.47	120.44	117.70
1	AA	1196	A	C4-C5-C6	5.47	119.74	117.00
1	AA	1012	A	N9-C4-C5	5.47	107.99	105.80
22	BA	430	A	N3-C4-N9	5.47	131.78	127.40
22	BA	2516	A	N3-C4-N9	5.47	131.78	127.40
22	BA	2682	A	N3-C4-N9	5.47	131.78	127.40
1	AA	223	A	N3-C4-N9	5.47	131.77	127.40
1	AA	1251	A	C4-C5-N7	-5.47	107.97	110.70
22	BA	751	A	C4-C5-N7	-5.47	107.97	110.70
22	BA	1745	A	N3-C4-N9	5.47	131.78	127.40
22	BA	2000	C	N3-C2-O2	-5.47	118.07	121.90
1	AA	120	A	C4-C5-C6	5.47	119.73	117.00
1	AA	353	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	454	G	N3-C4-C5	-5.47	125.87	128.60
22	BA	1755	A	C4-C5-N7	-5.47	107.97	110.70
22	BA	2281	A	C5-C6-N1	5.47	120.43	117.70
1	AA	1329	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1480	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	347	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	727	A	N3-C4-N9	5.46	131.77	127.40
22	BA	1609	A	N9-C4-C5	5.46	107.99	105.80
22	BA	2761	A	C5-C6-N1	5.46	120.43	117.70
22	BA	1264	A	C4-C5-C6	5.46	119.73	117.00
22	BA	1784	A	N9-C4-C5	5.46	107.98	105.80
22	BA	2054	A	C5-C6-N1	5.46	120.43	117.70
1	AA	1254	A	N3-C4-N9	5.46	131.77	127.40
1	AA	1333	A	N3-C4-N9	5.46	131.77	127.40
22	BA	167	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	943	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	109	A	C5-N7-C8	5.46	106.63	103.90
1	AA	1082	A	N3-C4-N9	5.46	131.76	127.40
22	BA	74	A	C4-C5-C6	5.46	119.73	117.00
22	BA	1847	A	C5-C6-N1	5.46	120.43	117.70
22	BA	1987	A	C4-C5-C6	5.46	119.73	117.00
22	BA	1987	A	C5-C6-N1	5.46	120.43	117.70
22	BA	2733	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	2734	A	N3-C4-N9	5.46	131.76	127.40
1	AA	596	A	C4-C5-C6	5.46	119.73	117.00
22	BA	1084	A	C4-C5-N7	-5.45	107.97	110.70
22	BA	1194	A	C5-C6-N1	5.45	120.43	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1614	A	C4-C5-N7	-5.45	107.97	110.70
22	BA	1805	A	C4-C5-N7	-5.45	107.97	110.70
22	BA	2542	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	969	A	C4-C5-N7	-5.45	107.97	110.70
22	BA	1745	A	N9-C4-C5	5.45	107.98	105.80
22	BA	1853	A	C5-C6-N1	5.45	120.43	117.70
22	BA	1977	A	C8-N9-C4	5.45	107.98	105.80
1	AA	19	A	C4-C5-N7	-5.45	107.98	110.70
3	AC	84	VAL	CG1-CB-CG2	-5.45	102.18	110.90
22	BA	347	A	N3-C4-N9	5.45	131.76	127.40
22	BA	821	A	C4-C5-N7	-5.45	107.97	110.70
22	BA	2879	A	N9-C4-C5	5.45	107.98	105.80
1	AA	72	A	C5-C6-N1	5.45	120.42	117.70
1	AA	1456	A	C4-C5-N7	-5.45	107.98	110.70
22	BA	272	A	N3-C4-N9	5.45	131.76	127.40
22	BA	603	A	C4-C5-C6	5.45	119.72	117.00
22	BA	1701	A	C4-C5-N7	-5.45	107.98	110.70
22	BA	1916	A	N3-C4-N9	5.45	131.76	127.40
1	AA	466	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	1410	A	C5-C6-N1	5.44	120.42	117.70
55	B8	21	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	109	A	N9-C4-C5	5.44	107.98	105.80
1	AA	1110	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	430	A	N3-C4-N9	5.44	131.75	127.40
1	AA	432	A	N3-C4-N9	5.44	131.75	127.40
22	BA	1095	A	N3-C4-N9	5.44	131.75	127.40
22	BA	2856	A	C5-C6-N1	5.44	120.42	117.70
1	AA	1225	A	N3-C4-N9	5.44	131.75	127.40
1	AA	1357	A	N3-C4-N9	5.44	131.75	127.40
22	BA	324	A	N3-C4-N9	5.44	131.75	127.40
22	BA	1286	A	C5-C6-N1	5.44	120.42	117.70
1	AA	1145	A	C4-C5-C6	5.44	119.72	117.00
22	BA	443	A	C4-C5-N7	-5.44	107.98	110.70
22	BA	541	A	N3-C4-N9	5.44	131.75	127.40
1	AA	336	A	C4-C5-C6	5.43	119.72	117.00
22	BA	1268	A	N3-C4-N9	5.43	131.75	127.40
23	BB	58	A	C4-C5-N7	-5.43	107.98	110.70
22	BA	231	A	C5-C6-N1	5.43	120.42	117.70
22	BA	750	A	N9-C4-C5	5.43	107.97	105.80
22	BA	2590	A	C4-C5-N7	-5.43	107.98	110.70
23	BB	50	A	N3-C4-N9	5.43	131.75	127.40
1	AA	95	C	C2-N1-C1'	5.43	124.77	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	165	A	C4-C5-C6	5.43	119.71	117.00
22	BA	933	A	N9-C4-C5	5.43	107.97	105.80
22	BA	2706	A	N3-C4-N9	5.43	131.74	127.40
1	AA	72	A	N3-C4-N9	5.43	131.74	127.40
22	BA	272	A	C5-C6-N1	5.43	120.41	117.70
22	BA	460	A	N9-C4-C5	5.43	107.97	105.80
1	AA	432	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	546	A	C4-C5-N7	-5.43	107.99	110.70
22	BA	219	A	N3-C4-N9	5.43	131.74	127.40
22	BA	1987	A	N3-C4-N9	5.43	131.74	127.40
1	AA	78	A	N9-C4-C5	5.42	107.97	105.80
1	AA	1101	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	1216	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	1805	A	N3-C4-N9	5.42	131.74	127.40
22	BA	2778	A	N3-C4-N9	5.42	131.74	127.40
1	AA	1152	A	N3-C4-N9	5.42	131.74	127.40
22	BA	608	A	C4-C5-C6	5.42	119.71	117.00
1	AA	98	A	N3-C4-N9	5.42	131.74	127.40
22	BA	195	A	C4-C5-C6	5.42	119.71	117.00
22	BA	346	A	C4-C5-C6	5.42	119.71	117.00
22	BA	2038	G	N1-C6-O6	-5.42	116.65	119.90
1	AA	197	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	2639	A	C4-C5-C6	5.42	119.71	117.00
1	AA	909	A	C4-C5-C6	5.42	119.71	117.00
1	AA	1036	A	N3-C4-N9	5.42	131.74	127.40
1	AA	205	A	N3-C4-N9	5.42	131.73	127.40
1	AA	694	A	N3-C4-N9	5.42	131.73	127.40
1	AA	908	A	N3-C4-N9	5.42	131.73	127.40
22	BA	1321	A	N3-C4-N9	5.42	131.73	127.40
22	BA	1876	A	N3-C4-N9	5.42	131.73	127.40
22	BA	2478	A	N3-C4-N9	5.42	131.73	127.40
22	BA	2560	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	590	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	2009	A	N3-C4-N9	5.42	131.73	127.40
1	AA	547	A	C4-C5-N7	-5.41	107.99	110.70
22	BA	2225	A	N9-C4-C5	5.41	107.97	105.80
1	AA	640	A	N3-C4-N9	5.41	131.73	127.40
22	BA	352	A	C4-C5-N7	-5.41	107.99	110.70
22	BA	2391	G	O4'-C1'-N9	5.41	112.53	108.20
22	BA	2810	A	C4-C5-C6	5.41	119.70	117.00
1	AA	315	A	C5-C6-N1	5.41	120.41	117.70
22	BA	1077	A	C4-C5-N7	-5.41	108.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1960	A	C4-C5-N7	-5.41	108.00	110.70
22	BA	1314	C	C2-N1-C1'	5.41	124.75	118.80
22	BA	1246	A	C4-C5-C6	5.41	119.70	117.00
22	BA	1885	A	N9-C4-C5	5.41	107.96	105.80
22	BA	2435	A	N3-C4-N9	5.41	131.72	127.40
22	BA	2634	A	C5-C6-N1	5.40	120.40	117.70
22	BA	1637	A	N3-C4-N9	5.40	131.72	127.40
1	AA	98	A	C5-C6-N1	5.40	120.40	117.70
1	AA	223	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	1176	A	N3-C4-N9	5.40	131.72	127.40
22	BA	1010	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	2459	A	C5-C6-N1	5.40	120.40	117.70
1	AA	435	A	N3-C4-N9	5.40	131.72	127.40
1	AA	1437	A	N3-C4-N9	5.40	131.72	127.40
22	BA	1453	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	1070	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	2727	A	N9-C4-C5	5.40	107.96	105.80
1	AA	120	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	509	A	C4-C5-N7	-5.39	108.00	110.70
22	BA	195	A	C5-C6-N1	5.39	120.40	117.70
22	BA	2054	A	C8-N9-C4	5.39	107.96	105.80
22	BA	2314	A	C4-C5-C6	5.39	119.70	117.00
22	BA	2632	A	C4-C5-C6	5.39	119.70	117.00
1	AA	149	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	787	A	N9-C4-C5	5.39	107.96	105.80
1	AA	1252	A	N3-C4-N9	5.39	131.71	127.40
1	AA	1508	A	N3-C4-N9	5.39	131.72	127.40
22	BA	2134	A	C4-C5-N7	-5.39	108.00	110.70
22	BA	643	A	N3-C4-N9	5.39	131.71	127.40
22	BA	1069	A	C4-C5-N7	-5.39	108.00	110.70
22	BA	1272	A	C4-C5-C6	5.39	119.70	117.00
1	AA	1014	A	C4-C5-N7	-5.39	108.00	110.70
22	BA	144	A	N9-C4-C5	5.39	107.96	105.80
22	BA	716	A	C4-C5-C6	5.39	119.69	117.00
22	BA	1566	A	C4-C5-C6	5.39	119.69	117.00
22	BA	1654	A	C8-N9-C4	5.39	107.96	105.80
1	AA	784	A	C5-C6-N1	5.39	120.39	117.70
22	BA	819	A	C4-C5-N7	-5.39	108.01	110.70
1	AA	7	A	C4-C5-C6	5.39	119.69	117.00
22	BA	1785	A	C5-N7-C8	5.39	106.59	103.90
22	BA	2205	A	N3-C4-N9	5.39	131.71	127.40
22	BA	2317	A	C4-C5-N7	-5.39	108.01	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2369	A	N3-C4-N9	5.39	131.71	127.40
22	BA	2560	A	C5-C6-N1	5.39	120.39	117.70
22	BA	2560	A	N3-C4-N9	5.39	131.71	127.40
22	BA	2679	A	C5-C6-N1	5.39	120.39	117.70
22	BA	149	A	N3-C4-N9	5.38	131.71	127.40
22	BA	655	A	C4-C5-C6	5.38	119.69	117.00
22	BA	920	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	1569	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	532	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	1439	A	N3-C4-N9	5.38	131.71	127.40
22	BA	1569	A	C5-C6-N1	5.38	120.39	117.70
22	BA	1665	A	N9-C4-C5	5.38	107.95	105.80
23	BB	29	A	C4-C5-N7	-5.38	108.01	110.70
23	BB	45	A	N3-C4-N9	5.38	131.71	127.40
1	AA	7	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	205	G	O4'-C1'-N9	5.38	112.50	108.20
22	BA	556	A	C5-C6-N1	5.38	120.39	117.70
22	BA	1968	G	O5'-P-OP1	-5.38	100.86	105.70
1	AA	1225	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1269	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	1103	A	N3-C4-N9	5.38	131.70	127.40
22	BA	1392	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	2333	A	N9-C4-C5	5.38	107.95	105.80
1	AA	675	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	1912	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	2615	U	N3-C2-O2	-5.38	118.44	122.20
22	BA	2860	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	983	A	N9-C4-C5	5.38	107.95	105.80
22	BA	1679	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	2013	A	N3-C4-N9	5.38	131.70	127.40
22	BA	2826	A	N3-C4-N9	5.38	131.70	127.40
22	BA	95	A	N3-C4-N9	5.38	131.70	127.40
22	BA	900	A	N3-C4-N9	5.38	131.70	127.40
1	AA	1092	A	C4-C5-N7	-5.37	108.01	110.70
22	BA	749	A	N3-C4-N9	5.37	131.70	127.40
22	BA	782	A	C4-C5-N7	-5.37	108.01	110.70
22	BA	1069	A	C4-C5-C6	5.37	119.69	117.00
22	BA	1739	A	N3-C4-N9	5.37	131.70	127.40
22	BA	2468	A	N3-C4-N9	5.37	131.70	127.40
22	BA	2851	A	N9-C4-C5	5.37	107.95	105.80
1	AA	869	G	N1-C6-O6	-5.37	116.68	119.90
1	AA	946	A	C5-C6-N1	5.37	120.39	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	182	A	N3-C4-N9	5.37	131.70	127.40
22	BA	655	A	C8-N9-C4	5.37	107.95	105.80
22	BA	1802	A	C4-C5-N7	-5.37	108.01	110.70
22	BA	1080	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	1144	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	59	A	N3-C4-N9	5.37	131.69	127.40
1	AA	1019	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	190	A	N3-C4-N9	5.37	131.69	127.40
22	BA	735	A	N9-C4-C5	5.37	107.95	105.80
22	BA	1000	A	C4-C5-C6	5.37	119.69	117.00
22	BA	1932	A	N3-C4-N9	5.37	131.70	127.40
22	BA	807	U	N1-C2-N3	5.37	118.12	114.90
22	BA	1970	A	N3-C4-C5	-5.37	123.04	126.80
1	AA	182	A	C4-C5-C6	5.37	119.68	117.00
1	AA	579	A	N3-C4-N9	5.37	131.69	127.40
22	BA	71	A	N9-C4-C5	5.37	107.95	105.80
22	BA	572	A	C5-C6-N1	5.37	120.38	117.70
22	BA	2284	A	C5-C6-N1	5.37	120.38	117.70
22	BA	2564	A	C5-C6-N1	5.37	120.38	117.70
1	AA	655	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	2453	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	414	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	466	A	N3-C4-N9	5.36	131.69	127.40
22	BA	443	A	N3-C4-N9	5.36	131.69	127.40
23	BB	115	A	N3-C4-N9	5.36	131.69	127.40
22	BA	1872	A	N9-C4-C5	5.36	107.94	105.80
1	AA	454	G	N9-C4-C5	-5.36	103.26	105.40
7	AG	33	ASP	N-CA-CB	-5.36	100.95	110.60
22	BA	833	A	N3-C4-N9	5.36	131.69	127.40
22	BA	2058	A	N3-C4-N9	5.36	131.69	127.40
22	BA	2333	A	N3-C4-N9	5.36	131.69	127.40
22	BA	1327	A	N3-C4-N9	5.36	131.69	127.40
22	BA	2814	A	C5-N7-C8	5.36	106.58	103.90
1	AA	596	A	N3-C4-N9	5.35	131.68	127.40
22	BA	342	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	1248	A	C4-C5-N7	-5.35	108.02	110.70
55	B8	59	A	C4-C5-N7	-5.35	108.02	110.70
22	BA	345	A	N3-C4-N9	5.35	131.68	127.40
22	BA	141	G	O4'-C1'-N9	-5.35	103.92	108.20
22	BA	2418	A	N3-C4-N9	5.35	131.68	127.40
22	BA	2850	A	C4-C5-N7	-5.35	108.03	110.70
1	AA	1410	A	C4-C5-N7	-5.35	108.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1476	A	C4-C5-N7	-5.35	108.03	110.70
22	BA	172	A	C4-C5-N7	-5.35	108.03	110.70
22	BA	829	A	C4-C5-C6	5.35	119.67	117.00
55	B8	51	A	C5-C6-N1	5.35	120.37	117.70
22	BA	173	A	C5-C6-N1	5.35	120.37	117.70
22	BA	1640	A	C4-C5-C6	5.35	119.67	117.00
1	AA	635	A	N3-C4-N9	5.34	131.68	127.40
22	BA	127	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	492	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	1637	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	1093	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	2	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	53	A	N3-C4-N9	5.34	131.67	127.40
1	AA	573	A	N3-C4-N9	5.34	131.67	127.40
1	AA	1502	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	428	A	C8-N9-C4	5.34	107.94	105.80
22	BA	522	A	C5-C6-N1	5.34	120.37	117.70
22	BA	556	A	N9-C4-C5	5.34	107.94	105.80
22	BA	1759	A	N9-C4-C5	5.34	107.94	105.80
22	BA	2617	U	N3-C2-O2	-5.34	118.46	122.20
1	AA	172	A	C4-C5-C6	5.34	119.67	117.00
1	AA	1152	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	125	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	146	A	C5-C6-N1	5.34	120.37	117.70
22	BA	310	A	C5-C6-N1	5.34	120.37	117.70
22	BA	2052	A	N3-C4-N9	5.34	131.67	127.40
22	BA	2297	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	2322	A	N3-C4-N9	5.34	131.67	127.40
22	BA	2388	A	N9-C4-C5	5.34	107.94	105.80
22	BA	221	A	C5-C6-N1	5.33	120.37	117.70
29	BH	32	PRO	CA-N-CD	-5.33	104.03	111.50
1	AA	356	A	C5-C6-N1	5.33	120.37	117.70
22	BA	1383	A	C5-C6-N1	5.33	120.37	117.70
22	BA	1535	A	N3-C4-N9	5.33	131.67	127.40
22	BA	1994	C	C6-N1-C2	-5.33	118.17	120.30
22	BA	2135	A	N3-C4-N9	5.33	131.67	127.40
55	B8	38	A	C5-C6-N1	5.33	120.37	117.70
1	AA	196	A	C4-C5-N7	-5.33	108.03	110.70
22	BA	582	A	C5-C6-N1	5.33	120.36	117.70
22	BA	1000	A	N3-C4-N9	5.33	131.66	127.40
22	BA	1027	A	N3-C4-N9	5.33	131.67	127.40
1	AA	109	A	N3-C4-N9	5.33	131.66	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2564	A	N3-C4-N9	5.33	131.66	127.40
22	BA	2848	G	O4'-C1'-N9	5.33	112.46	108.20
1	AA	574	A	C4-C5-C6	5.33	119.67	117.00
1	AA	935	A	N3-C4-N9	5.33	131.66	127.40
22	BA	626	A	C5-N7-C8	5.33	106.56	103.90
22	BA	1032	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	8	A	C4-C5-C6	5.33	119.66	117.00
22	BA	1666	G	O5'-P-OP1	-5.33	100.91	105.70
22	BA	2126	A	N3-C4-N9	5.33	131.66	127.40
55	B8	42	A	N9-C4-C5	5.33	107.93	105.80
1	AA	913	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	1368	A	C4-C5-N7	-5.33	108.04	110.70
22	BA	127	A	C4-C5-C6	5.33	119.66	117.00
22	BA	430	A	N9-C4-C5	5.33	107.93	105.80
22	BA	973	A	C5-N7-C8	5.33	106.56	103.90
22	BA	1938	A	N3-C4-N9	5.33	131.66	127.40
22	BA	2051	A	C4-C5-N7	-5.33	108.04	110.70
22	BA	2564	A	C4-C5-C6	5.33	119.66	117.00
1	AA	53	A	C5-C6-N1	5.32	120.36	117.70
1	AA	621	A	N3-C4-N9	5.32	131.66	127.40
22	BA	49	A	N3-C4-N9	5.32	131.66	127.40
22	BA	207	A	N3-C4-N9	5.32	131.66	127.40
1	AA	1145	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	492	A	N3-C4-N9	5.32	131.66	127.40
22	BA	2679	A	N9-C4-C5	5.32	107.93	105.80
22	BA	2052	A	N9-C4-C5	5.32	107.93	105.80
22	BA	2439	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	2851	A	N3-C4-N9	5.32	131.66	127.40
1	AA	873	A	N9-C4-C5	5.32	107.93	105.80
1	AA	1229	A	N3-C4-N9	5.32	131.66	127.40
22	BA	472	A	N3-C4-N9	5.32	131.65	127.40
1	AA	181	A	C8-N9-C4	5.32	107.93	105.80
1	AA	618	C	C5-C4-N4	5.32	123.92	120.20
1	AA	938	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	1103	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	1214	A	C5-C6-N1	5.32	120.36	117.70
22	BA	1755	A	C4-C5-C6	5.32	119.66	117.00
22	BA	1936	A	C8-N9-C1'	-5.32	118.13	127.70
22	BA	2418	A	N9-C4-C5	5.32	107.93	105.80
22	BA	2547	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	2749	A	C4-C5-N7	-5.32	108.04	110.70
23	BB	94	A	C5-C6-N1	5.32	120.36	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	655	A	C4-C5-N7	-5.31	108.04	110.70
22	BA	1427	A	C4-C5-N7	-5.31	108.04	110.70
22	BA	2311	A	C4-C5-N7	-5.31	108.04	110.70
1	AA	694	A	C4-C5-N7	-5.31	108.04	110.70
22	BA	342	A	C4-C5-C6	5.31	119.66	117.00
22	BA	1246	A	C5-C6-N1	5.31	120.36	117.70
22	BA	2665	A	C4-C5-N7	-5.31	108.04	110.70
22	BA	1395	A	C4-C5-N7	-5.31	108.04	110.70
22	BA	1803	A	C5-C6-N1	5.31	120.36	117.70
22	BA	1966	A	N3-C4-N9	5.31	131.65	127.40
22	BA	2670	A	C8-N9-C4	5.31	107.92	105.80
1	AA	1004	A	C4-C5-N7	-5.31	108.05	110.70
22	BA	141	G	C5-C6-O6	-5.31	125.42	128.60
22	BA	244	A	C5-C6-N1	5.31	120.36	117.70
22	BA	729	G	N3-C4-C5	-5.31	125.94	128.60
22	BA	1787	A	C4-C5-N7	-5.31	108.05	110.70
22	BA	2393	U	N3-C2-O2	-5.31	118.48	122.20
1	AA	864	A	N3-C4-N9	5.31	131.65	127.40
1	AA	1271	A	N3-C4-N9	5.31	131.65	127.40
1	AA	1275	A	N3-C4-N9	5.31	131.65	127.40
22	BA	821	A	C4-C5-C6	5.31	119.65	117.00
23	BB	57	A	C4-C5-N7	-5.31	108.05	110.70
1	AA	630	A	N3-C4-N9	5.30	131.64	127.40
1	AA	1102	A	N3-C4-N9	5.30	131.64	127.40
22	BA	103	A	N3-C4-N9	5.30	131.64	127.40
22	BA	497	A	N3-C4-N9	5.30	131.64	127.40
22	BA	753	A	C4-C5-N7	-5.30	108.05	110.70
22	BA	1028	A	N3-C4-N9	5.30	131.64	127.40
22	BA	1269	A	N3-C4-N9	5.30	131.64	127.40
22	BA	1593	A	N3-C4-N9	5.30	131.64	127.40
22	BA	2097	A	N9-C4-C5	5.30	107.92	105.80
1	AA	336	A	C4-C5-N7	-5.30	108.05	110.70
22	BA	1005	C	C6-N1-C2	-5.30	118.18	120.30
1	AA	119	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	435	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	1288	A	N3-C4-N9	5.30	131.64	127.40
22	BA	1080	A	N3-C4-N9	5.30	131.64	127.40
22	BA	1717	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	10	A	N3-C4-N9	5.30	131.64	127.40
1	AA	468	A	C4-C5-N7	-5.30	108.05	110.70
22	BA	1126	A	N3-C4-N9	5.30	131.64	127.40
22	BA	2163	A	N3-C4-N9	5.30	131.64	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2340	A	C5-C6-N1	5.30	120.35	117.70
23	BB	75	G	N3-C4-C5	-5.30	125.95	128.60
1	AA	152	A	C5-C6-N1	5.30	120.35	117.70
1	AA	816	A	N3-C4-N9	5.30	131.64	127.40
22	BA	91	A	C4-C5-N7	-5.30	108.05	110.70
22	BA	838	C	N3-C2-O2	-5.30	118.19	121.90
22	BA	1069	A	C8-N9-C4	5.30	107.92	105.80
22	BA	1393	A	C4-C5-C6	5.30	119.65	117.00
22	BA	2099	U	O4'-C1'-N1	5.30	112.44	108.20
1	AA	155	A	N3-C4-N9	5.29	131.64	127.40
1	AA	179	A	C4-C5-N7	-5.29	108.05	110.70
1	AA	1000	A	C5-C6-N1	5.29	120.35	117.70
22	BA	574	A	C4-C5-N7	-5.29	108.05	110.70
1	AA	174	A	N3-C4-N9	5.29	131.63	127.40
22	BA	342	A	C5-C6-N1	5.29	120.35	117.70
22	BA	1548	A	C4-C5-C6	5.29	119.65	117.00
22	BA	1622	G	N3-C4-N9	5.29	129.18	126.00
22	BA	1970	A	C6-N1-C2	5.29	121.78	118.60
22	BA	2065	C	C6-N1-C2	-5.29	118.18	120.30
22	BA	2071	A	C4-C5-N7	-5.29	108.05	110.70
23	BB	59	A	N9-C4-C5	5.29	107.92	105.80
1	AA	1081	A	C5-C6-N1	5.29	120.35	117.70
22	BA	1570	A	C4-C5-N7	-5.29	108.05	110.70
1	AA	787	A	N3-C4-N9	5.29	131.63	127.40
54	B7	9	A	C4-C5-C6	5.29	119.64	117.00
22	BA	1367	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	2212	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	126	A	C4-C5-C6	5.29	119.64	117.00
22	BA	344	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	1783	A	C4-C5-C6	5.29	119.64	117.00
1	AA	411	A	C5-C6-N1	5.29	120.34	117.70
1	AA	1157	A	C5-C6-N1	5.29	120.34	117.70
22	BA	981	A	C4-C5-C6	5.29	119.64	117.00
22	BA	1978	A	C8-N9-C4	5.29	107.91	105.80
22	BA	2314	A	C5-C6-N1	5.29	120.34	117.70
22	BA	2541	A	C4-C5-N7	-5.29	108.06	110.70
1	AA	1044	A	C5-C6-N1	5.28	120.34	117.70
1	AA	1368	A	N3-C4-N9	5.28	131.63	127.40
1	AA	1502	A	C4-C5-C6	5.28	119.64	117.00
22	BA	149	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	1635	A	N3-C4-N9	5.28	131.63	127.40
1	AA	353	A	C5-C6-N1	5.28	120.34	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	715	A	N3-C4-N9	5.28	131.62	127.40
22	BA	1552	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	1936	A	C5-N7-C8	5.28	106.54	103.90
22	BA	2541	A	N3-C4-N9	5.28	131.62	127.40
22	BA	2579	C	O5'-P-OP1	-5.28	100.95	105.70
1	AA	533	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	1101	A	C4-C5-C6	5.28	119.64	117.00
1	AA	1446	A	C5-C6-N1	5.28	120.34	117.70
22	BA	2430	A	C6-N1-C2	5.28	121.77	118.60
1	AA	441	A	N3-C4-N9	5.28	131.62	127.40
22	BA	608	A	N9-C4-C5	5.28	107.91	105.80
22	BA	1634	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	1700	A	N9-C4-C5	5.28	107.91	105.80
1	AA	441	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	470	C	C6-N1-C2	-5.28	118.19	120.30
22	BA	1048	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	1342	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	1505	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	1655	A	C5-C6-N1	5.28	120.34	117.70
22	BA	2184	A	N3-C4-N9	5.28	131.62	127.40
22	BA	246	C	C6-N1-C2	-5.27	118.19	120.30
22	BA	453	A	N9-C4-C5	5.27	107.91	105.80
22	BA	899	A	C4-C5-N7	-5.27	108.06	110.70
22	BA	1014	A	N3-C4-N9	5.27	131.62	127.40
22	BA	1586	A	N3-C4-N9	5.27	131.62	127.40
22	BA	1877	A	N3-C4-N9	5.27	131.62	127.40
22	BA	2602	A	C4-C5-N7	-5.27	108.06	110.70
22	BA	2711	A	N3-C4-N9	5.27	131.62	127.40
1	AA	794	A	N3-C4-N9	5.27	131.62	127.40
1	AA	1005	A	N3-C4-N9	5.27	131.62	127.40
22	BA	1969	A	N3-C4-N9	5.27	131.62	127.40
22	BA	2893	A	N3-C4-N9	5.27	131.62	127.40
1	AA	263	A	C4-C5-N7	-5.27	108.07	110.70
1	AA	356	A	C4-C5-N7	-5.27	108.07	110.70
22	BA	2809	A	N3-C4-N9	5.27	131.61	127.40
22	BA	1730	C	N1-C2-O2	5.27	122.06	118.90
1	AA	280	C	C6-N1-C2	5.26	122.41	120.30
1	AA	602	A	N3-C4-N9	5.26	131.61	127.40
1	AA	1418	A	N9-C4-C5	5.26	107.91	105.80
1	AA	1437	A	N9-C4-C5	5.26	107.91	105.80
22	BA	572	A	N9-C4-C5	5.26	107.91	105.80
22	BA	1784	A	C4-C5-N7	-5.26	108.07	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2386	A	N3-C4-N9	5.26	131.61	127.40
22	BA	1008	A	C4-C5-C6	5.26	119.63	117.00
22	BA	1569	A	C4-C5-C6	5.26	119.63	117.00
1	AA	845	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	332	A	C5-C6-N1	5.26	120.33	117.70
22	BA	477	A	N9-C4-C5	5.26	107.90	105.80
22	BA	502	A	C4-C5-C6	5.26	119.63	117.00
22	BA	1253	A	C5-N7-C8	5.26	106.53	103.90
22	BA	2547	A	C5-C6-N1	5.26	120.33	117.70
22	BA	2736	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	640	A	C5-C6-N1	5.26	120.33	117.70
22	BA	505	A	N3-C4-N9	5.26	131.61	127.40
22	BA	2810	A	C5-C6-N1	5.26	120.33	117.70
1	AA	470	C	C2-N1-C1'	5.26	124.58	118.80
1	AA	768	A	N3-C4-N9	5.26	131.60	127.40
1	AA	1396	A	C5-C6-N1	5.26	120.33	117.70
22	BA	222	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	2430	A	C5'-C4'-O4'	5.26	115.41	109.10
22	BA	2516	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	559	A	N3-C4-N9	5.25	131.60	127.40
22	BA	114	U	C2-N1-C1'	5.25	124.01	117.70
22	BA	1272	A	C8-N9-C4	5.25	107.90	105.80
23	BB	104	A	N3-C4-N9	5.25	131.60	127.40
22	BA	118	A	C4-C5-C6	5.25	119.63	117.00
22	BA	2497	A	N3-C4-N9	5.25	131.60	127.40
22	BA	233	A	N9-C4-C5	5.25	107.90	105.80
22	BA	718	A	N3-C4-N9	5.25	131.60	127.40
22	BA	1591	A	N9-C4-C5	5.25	107.90	105.80
22	BA	1655	A	N3-C4-N9	5.25	131.60	127.40
1	AA	195	A	C4-C5-C6	5.25	119.62	117.00
1	AA	243	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	689	A	C5-C6-N1	5.25	120.32	117.70
22	BA	1616	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	2267	A	C5-C6-N1	5.25	120.32	117.70
1	AA	499	A	N3-C4-N9	5.25	131.60	127.40
1	AA	642	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	71	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	1603	A	N9-C4-C5	5.25	107.90	105.80
22	BA	2036	C	C6-N1-C2	-5.25	118.20	120.30
55	B8	42	A	C4-C5-N7	-5.25	108.08	110.70
1	AA	181	A	N3-C4-N9	5.25	131.60	127.40
22	BA	2425	A	C4-C5-N7	-5.25	108.08	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	151	A	C5-C6-N1	5.24	120.32	117.70
1	AA	309	A	C5-C6-N1	5.24	120.32	117.70
22	BA	2340	A	C8-N9-C4	5.24	107.90	105.80
22	BA	621	A	C4-C5-C6	5.24	119.62	117.00
1	AA	366	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	815	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	1024	G	O4'-C1'-N9	5.24	112.39	108.20
1	AA	1360	A	N3-C4-N9	5.24	131.59	127.40
22	BA	279	A	C5-C6-N1	5.24	120.32	117.70
22	BA	866	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	1580	A	N3-C4-N9	5.24	131.59	127.40
22	BA	1821	A	C4-C5-C6	5.24	119.62	117.00
22	BA	1981	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	199	A	C5-C6-N1	5.24	120.32	117.70
1	AA	1256	A	N3-C4-N9	5.24	131.59	127.40
22	BA	2191	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	1067	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	1383	A	C4-C5-C6	5.24	119.62	117.00
55	B8	73	A	C5-C6-N1	5.23	120.32	117.70
1	AA	80	A	N3-C4-N9	5.23	131.58	127.40
1	AA	1111	A	C4-C5-N7	-5.23	108.08	110.70
22	BA	1791	A	C4-C5-N7	-5.23	108.08	110.70
22	BA	2062	A	C4-C5-N7	-5.23	108.09	110.70
22	BA	2184	A	C5-C6-N1	5.23	120.31	117.70
1	AA	78	A	C5-C6-N1	5.23	120.31	117.70
1	AA	743	A	C5-C6-N1	5.23	120.31	117.70
1	AA	1320	C	N1-C2-N3	-5.23	115.54	119.20
22	BA	371	A	C4-C5-N7	-5.23	108.09	110.70
22	BA	603	A	C8-N9-C4	5.23	107.89	105.80
22	BA	673	C	N1-C2-O2	-5.23	115.76	118.90
22	BA	2005	A	N3-C4-N9	5.23	131.58	127.40
1	AA	192	A	N3-C4-N9	5.23	131.58	127.40
22	BA	706	A	N3-C4-N9	5.23	131.58	127.40
22	BA	1367	A	N3-C4-N9	5.22	131.58	127.40
22	BA	1496	A	N3-C4-N9	5.22	131.58	127.40
22	BA	2449	U	C5-C4-O4	-5.22	122.77	125.90
22	BA	2589	A	N3-C4-N9	5.22	131.58	127.40
22	BA	670	A	N3-C4-N9	5.22	131.58	127.40
1	AA	303	A	C5-C6-N1	5.22	120.31	117.70
22	BA	1084	A	N3-C4-N9	5.22	131.58	127.40
22	BA	2734	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	706	A	C4-C5-N7	-5.22	108.09	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	825	A	C5-C6-N1	5.22	120.31	117.70
22	BA	715	A	C8-N9-C4	5.22	107.89	105.80
22	BA	980	A	C5-C6-N1	5.22	120.31	117.70
22	BA	1050	A	C4-C5-N7	-5.22	108.09	110.70
23	BB	58	A	N3-C4-N9	5.22	131.58	127.40
22	BA	282	A	C8-N9-C4	5.22	107.89	105.80
22	BA	1746	A	N3-C4-N9	5.22	131.57	127.40
22	BA	2448	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	171	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	1590	A	N3-C4-N9	5.22	131.57	127.40
22	BA	2412	A	N3-C4-N9	5.22	131.57	127.40
1	AA	411	A	N3-C4-N9	5.21	131.57	127.40
1	AA	802	A	C4-C5-N7	-5.21	108.09	110.70
1	AA	1155	A	N3-C4-N9	5.21	131.57	127.40
1	AA	1441	A	C8-N9-C4	5.21	107.89	105.80
22	BA	5	A	C5-C6-N1	5.21	120.31	117.70
22	BA	1322	A	N9-C4-C5	5.21	107.89	105.80
55	B8	73	A	C4-C5-N7	-5.21	108.09	110.70
22	BA	103	A	C4-C5-N7	-5.21	108.09	110.70
22	BA	250	G	C5-C6-O6	5.21	131.73	128.60
22	BA	1189	A	C4-C5-N7	-5.21	108.09	110.70
1	AA	695	A	N3-C4-N9	5.21	131.57	127.40
22	BA	176	A	C5-C6-N1	5.21	120.31	117.70
22	BA	177	G	O4'-C1'-N9	5.21	112.37	108.20
22	BA	368	A	N3-C4-N9	5.21	131.57	127.40
22	BA	1413	A	N3-C4-N9	5.21	131.57	127.40
22	BA	1759	A	C8-N9-C4	5.21	107.89	105.80
22	BA	1780	A	C4-C5-N7	-5.21	108.09	110.70
22	BA	1901	A	N3-C4-N9	5.21	131.57	127.40
22	BA	503	A	N3-C4-N9	5.21	131.57	127.40
1	AA	825	A	C4-C5-N7	-5.21	108.10	110.70
1	AA	915	A	C8-N9-C4	5.21	107.88	105.80
22	BA	1544	A	C5-C6-N1	5.21	120.30	117.70
1	AA	937	A	N3-C4-N9	5.21	131.56	127.40
22	BA	324	A	N9-C4-C5	5.21	107.88	105.80
22	BA	2273	A	C4-C5-N7	-5.21	108.10	110.70
1	AA	1150	A	C4-C5-N7	-5.21	108.10	110.70
22	BA	2468	A	C5-C6-N1	5.21	120.30	117.70
1	AA	26	A	C4-C5-N7	-5.20	108.10	110.70
1	AA	901	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	666	A	N9-C4-C5	5.20	107.88	105.80
22	BA	844	A	N3-C4-N9	5.20	131.56	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2340	A	N9-C4-C5	5.20	107.88	105.80
22	BA	2900	A	C5-C6-N1	5.20	120.30	117.70
55	B8	20	U	C4-C5-C6	-5.20	116.58	119.70
22	BA	909	A	C4-C5-C6	5.20	119.60	117.00
22	BA	1583	A	C4-C5-N7	-5.20	108.10	110.70
1	AA	81	A	C4-C5-N7	-5.20	108.10	110.70
1	AA	349	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	900	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	920	A	N3-C4-N9	5.20	131.56	127.40
22	BA	1359	A	C5-C6-N1	5.20	120.30	117.70
22	BA	1749	A	N3-C4-N9	5.20	131.56	127.40
22	BA	2134	A	N3-C4-N9	5.20	131.56	127.40
22	BA	2190	G	C8-N9-C4	-5.20	104.32	106.40
41	BT	1	MET	CA-C-N	-5.20	105.76	117.20
1	AA	143	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	2080	A	C4-C5-N7	-5.20	108.10	110.70
1	AA	629	A	N3-C4-N9	5.20	131.56	127.40
22	BA	1057	A	N3-C4-N9	5.20	131.56	127.40
1	AA	489	C	C2-N1-C1'	5.20	124.52	118.80
1	AA	1035	A	C4-C5-N7	-5.20	108.10	110.70
1	AA	1196	A	C8-N9-C4	5.20	107.88	105.80
1	AA	1311	A	C5-C6-N1	5.20	120.30	117.70
22	BA	1378	A	C5-C6-N1	5.20	120.30	117.70
22	BA	1900	A	N3-C4-N9	5.20	131.56	127.40
55	B8	41	A	C4-C5-N7	-5.20	108.10	110.70
1	AA	383	A	C6-C5-N7	-5.19	128.67	132.30
1	AA	665	A	C4-C5-N7	-5.19	108.11	110.70
1	AA	1229	A	C5-C6-N1	5.19	120.30	117.70
22	BA	279	A	C4-C5-C6	5.19	119.59	117.00
22	BA	877	A	C4-C5-N7	-5.19	108.11	110.70
1	AA	546	A	N3-C4-N9	5.19	131.55	127.40
1	AA	1413	A	C4-C5-N7	-5.19	108.11	110.70
4	AD	64	ILE	CG1-CB-CG2	-5.19	99.99	111.40
22	BA	453	A	C5-C6-N1	5.19	120.29	117.70
22	BA	1328	A	C4-C5-N7	-5.19	108.11	110.70
22	BA	1469	A	C4-C5-N7	-5.19	108.11	110.70
22	BA	1088	A	C4-C5-N7	-5.19	108.11	110.70
22	BA	1230	A	N3-C4-N9	5.19	131.55	127.40
1	AA	66	A	C4-C5-N7	-5.18	108.11	110.70
1	AA	371	A	C5-C6-N1	5.18	120.29	117.70
22	BA	94	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	412	A	N3-C4-N9	5.18	131.55	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	959	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	2212	A	N3-C4-N9	5.18	131.55	127.40
23	BB	109	A	C4-C5-N7	-5.18	108.11	110.70
1	AA	1447	A	N9-C4-C5	5.18	107.87	105.80
22	BA	675	A	N3-C4-N9	5.18	131.55	127.40
22	BA	1301	A	N3-C4-N9	5.18	131.55	127.40
22	BA	2071	A	N3-C4-N9	5.18	131.55	127.40
22	BA	2670	A	C5-C6-N1	5.18	120.29	117.70
22	BA	2792	A	C5-C6-N1	5.18	120.29	117.70
23	BB	119	A	C5-C6-N1	5.18	120.29	117.70
1	AA	315	A	N3-C4-N9	5.18	131.54	127.40
22	BA	1522	A	C4-C5-C6	5.18	119.59	117.00
22	BA	1626	A	N9-C4-C5	5.18	107.87	105.80
1	AA	8	A	C4-C5-N7	-5.18	108.11	110.70
1	AA	250	A	N3-C4-N9	5.18	131.54	127.40
1	AA	1151	A	N3-C4-N9	5.18	131.54	127.40
1	AA	1340	A	N9-C4-C5	5.18	107.87	105.80
22	BA	309	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	988	A	N3-C4-N9	5.18	131.54	127.40
22	BA	2170	A	N3-C4-N9	5.18	131.54	127.40
22	BA	2211	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	2288	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	928	A	C4-C5-N7	-5.18	108.11	110.70
1	AA	1483	A	N9-C4-C5	5.18	107.87	105.80
22	BA	227	A	N3-C4-N9	5.18	131.54	127.40
22	BA	789	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	1021	A	N9-C4-C5	5.18	107.87	105.80
22	BA	1495	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	1609	A	C8-N9-C4	5.18	107.87	105.80
22	BA	2037	A	N3-C4-N9	5.18	131.54	127.40
55	B8	58	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	1039	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	2317	A	N3-C4-N9	5.17	131.54	127.40
22	BA	2867	G	O4'-C1'-N9	5.17	112.34	108.20
22	BA	2886	A	N9-C4-C5	5.17	107.87	105.80
1	AA	309	A	C4-C5-C6	5.17	119.59	117.00
1	AA	1349	A	N3-C4-N9	5.17	131.54	127.40
55	B8	58	A	C4-C5-C6	5.17	119.59	117.00
1	AA	608	A	C5-C6-N1	5.17	120.29	117.70
1	AA	825	A	N3-C4-N9	5.17	131.54	127.40
1	AA	1180	A	N3-C4-N9	5.17	131.54	127.40
22	BA	429	A	C4-C5-N7	-5.17	108.11	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	863	A	C5-C6-N1	5.17	120.29	117.70
22	BA	1439	A	C5-C6-N1	5.17	120.29	117.70
22	BA	1509	A	N3-C4-N9	5.17	131.54	127.40
1	AA	579	A	C4-C5-N7	-5.17	108.12	110.70
22	BA	181	A	N3-C4-N9	5.17	131.53	127.40
22	BA	1632	A	N3-C4-N9	5.17	131.53	127.40
1	AA	777	A	C4-C5-C6	5.17	119.58	117.00
1	AA	1155	A	C5-C6-N1	5.17	120.28	117.70
1	AA	1250	A	C4-C5-N7	-5.17	108.12	110.70
1	AA	1288	A	C5-C6-N1	5.17	120.28	117.70
22	BA	119	A	C5-C6-N1	5.17	120.28	117.70
22	BA	2887	A	N3-C4-N9	5.17	131.53	127.40
1	AA	1227	A	C5-N7-C8	5.16	106.48	103.90
22	BA	761	A	C5-N7-C8	5.16	106.48	103.90
22	BA	1090	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	2241	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	2453	A	N3-C4-N9	5.16	131.53	127.40
22	BA	2600	A	N9-C4-C5	5.16	107.87	105.80
22	BA	2632	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	2675	A	N9-C4-C5	5.16	107.87	105.80
22	BA	2761	A	N3-C4-N9	5.16	131.53	127.40
22	BA	2823	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	189	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	1675	C	C6-N1-C2	-5.16	118.24	120.30
22	BA	1808	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	1866	A	N3-C4-N9	5.16	131.53	127.40
22	BA	1938	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	19	A	N3-C4-N9	5.16	131.53	127.40
22	BA	340	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	428	A	N9-C4-C5	5.16	107.86	105.80
22	BA	1508	A	N3-C4-N9	5.16	131.53	127.40
22	BA	1759	A	C5-C6-N1	5.16	120.28	117.70
22	BA	2823	A	N3-C4-N9	5.16	131.53	127.40
1	AA	430	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	348	A	C5-C6-N1	5.16	120.28	117.70
1	AA	415	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	482	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	596	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	412	A	N9-C4-C5	5.16	107.86	105.80
22	BA	515	A	C5-C6-N1	5.16	120.28	117.70
22	BA	739	A	N3-C4-N9	5.16	131.52	127.40
22	BA	1678	A	N3-C4-N9	5.16	131.53	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1858	A	C5-C6-N1	5.16	120.28	117.70
22	BA	2328	A	N3-C4-N9	5.16	131.53	127.40
55	B8	59	A	C5-C6-N1	5.16	120.28	117.70
1	AA	1492	A	C4-C5-N7	-5.15	108.12	110.70
22	BA	1307	A	N3-C4-N9	5.15	131.52	127.40
22	BA	2247	A	C4-C5-N7	-5.15	108.12	110.70
22	BA	2541	A	C4-C5-C6	5.15	119.58	117.00
54	B7	7	U	P-O3'-C3'	5.15	125.88	119.70
1	AA	101	A	C5-C6-N1	5.15	120.28	117.70
22	BA	972	A	N3-C4-N9	5.15	131.52	127.40
22	BA	1762	A	C4-C5-N7	-5.15	108.12	110.70
22	BA	1772	A	N3-C4-N9	5.15	131.52	127.40
22	BA	1838	C	C6-N1-C2	-5.15	118.24	120.30
1	AA	1275	A	C4-C5-N7	-5.15	108.12	110.70
22	BA	2009	A	C5-C6-N1	5.15	120.28	117.70
22	BA	2154	A	C4-C5-N7	-5.15	108.12	110.70
22	BA	2184	A	C4-C5-N7	-5.15	108.12	110.70
1	AA	915	A	C4-C5-N7	-5.15	108.13	110.70
22	BA	330	A	N9-C4-C5	5.15	107.86	105.80
22	BA	354	A	C4-C5-N7	-5.15	108.13	110.70
22	BA	428	A	N3-C4-N9	5.15	131.52	127.40
22	BA	1322	A	C8-N9-C4	5.15	107.86	105.80
22	BA	2266	A	C4-C5-C6	5.15	119.57	117.00
23	BB	78	A	C4-C5-N7	-5.15	108.13	110.70
1	AA	189	A	N3-C4-N9	5.15	131.52	127.40
22	BA	2809	A	C8-N9-C4	5.15	107.86	105.80
1	AA	282	A	C4-C5-N7	-5.14	108.13	110.70
1	AA	1213	A	C4-C5-C6	5.14	119.57	117.00
22	BA	789	A	N3-C4-N9	5.14	131.51	127.40
22	BA	1952	A	C8-N9-C4	5.14	107.86	105.80
23	BB	99	A	C4-C5-N7	-5.14	108.13	110.70
1	AA	1170	A	N9-C4-C5	5.14	107.86	105.80
22	BA	927	A	N3-C4-N9	5.14	131.51	127.40
22	BA	988	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	1189	A	C5-C6-N1	5.14	120.27	117.70
22	BA	2019	A	N3-C4-N9	5.14	131.51	127.40
22	BA	2163	A	O5'-P-OP1	-5.14	101.07	105.70
1	AA	602	A	C4-C5-N7	-5.14	108.13	110.70
1	AA	1008	U	O4'-C1'-N1	5.14	112.31	108.20
1	AA	1067	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	529	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	2378	A	N3-C4-N9	5.14	131.51	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	205	A	C4-C5-N7	-5.14	108.13	110.70
1	AA	288	A	C5-C6-N1	5.14	120.27	117.70
1	AA	1004	A	N3-C4-N9	5.14	131.51	127.40
22	BA	294	A	N9-C4-C5	5.14	107.86	105.80
22	BA	501	A	N3-C4-N9	5.14	131.51	127.40
22	BA	2542	A	C4-C5-C6	5.14	119.57	117.00
1	AA	344	A	C4-C5-N7	-5.14	108.13	110.70
1	AA	1146	A	N3-C4-N9	5.14	131.51	127.40
1	AA	1239	A	C5-C6-N1	5.14	120.27	117.70
22	BA	10	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	784	G	P-O3'-C3'	5.14	125.87	119.70
13	AM	19	LEU	CA-CB-CG	-5.14	103.48	115.30
22	BA	1395	A	C4-C5-C6	5.14	119.57	117.00
1	AA	270	A	C5-C6-N1	5.13	120.27	117.70
1	AA	306	A	N3-C4-N9	5.13	131.51	127.40
1	AA	1499	A	N3-C4-N9	5.13	131.51	127.40
22	BA	217	A	N3-C4-N9	5.13	131.51	127.40
22	BA	404	A	C4-C5-C6	5.13	119.57	117.00
22	BA	936	A	N3-C4-N9	5.13	131.51	127.40
22	BA	2003	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	2406	A	C5-C6-N1	5.13	120.27	117.70
22	BA	706	A	C4-C5-N7	-5.13	108.13	110.70
23	BB	34	A	N3-C4-N9	5.13	131.51	127.40
1	AA	535	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	996	A	C8-N9-C4	5.13	107.85	105.80
22	BA	1089	A	C4-C5-N7	-5.13	108.13	110.70
23	BB	119	A	N3-C4-N9	5.13	131.50	127.40
1	AA	130	A	C4-C5-N7	-5.13	108.14	110.70
1	AA	964	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	2366	A	C4-C5-N7	-5.13	108.14	110.70
1	AA	349	A	N3-C4-N9	5.13	131.50	127.40
1	AA	749	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	447	A	N3-C4-N9	5.13	131.50	127.40
22	BA	1596	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	972	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	1347	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	1885	A	N3-C4-N9	5.13	131.50	127.40
22	BA	2501	C	C5-C4-N4	5.13	123.79	120.20
1	AA	167	A	N3-C4-N9	5.12	131.50	127.40
22	BA	508	A	N3-C4-N9	5.12	131.50	127.40
22	BA	1858	A	N3-C4-N9	5.12	131.50	127.40
1	AA	1167	A	C4-C5-N7	-5.12	108.14	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1009	A	N3-C4-N9	5.12	131.50	127.40
22	BA	1254	A	N3-C4-N9	5.12	131.50	127.40
22	BA	1579	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	1346	A	C5-C6-N1	5.12	120.26	117.70
22	BA	84	A	C5-C6-N1	5.12	120.26	117.70
22	BA	478	A	N3-C4-N9	5.12	131.50	127.40
22	BA	1522	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	2198	A	C4-C5-C6	5.12	119.56	117.00
22	BA	207	A	C5-C6-N1	5.12	120.26	117.70
22	BA	2476	A	N3-C4-N9	5.12	131.50	127.40
1	AA	949	A	N3-C4-N9	5.12	131.50	127.40
1	AA	496	A	N9-C4-C5	5.12	107.85	105.80
1	AA	1408	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	2094	A	N3-C4-N9	5.12	131.49	127.40
1	AA	814	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	1253	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	2270	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	572	A	C4-C5-C6	5.11	119.56	117.00
22	BA	910	A	N3-C4-N9	5.11	131.49	127.40
22	BA	1151	A	N9-C4-C5	5.11	107.85	105.80
22	BA	144	A	C8-N9-C4	5.11	107.84	105.80
22	BA	2288	A	N3-C4-N9	5.11	131.49	127.40
22	BA	2478	A	C5-C6-N1	5.11	120.26	117.70
1	AA	704	A	C5-C6-N1	5.11	120.25	117.70
1	AA	1500	A	C5-C6-N1	5.11	120.25	117.70
22	BA	294	A	N3-C4-N9	5.11	131.49	127.40
22	BA	1762	A	N3-C4-N9	5.11	131.49	127.40
1	AA	161	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	2128	G	N1-C6-O6	-5.11	116.83	119.90
22	BA	2199	A	C5-C6-N1	5.11	120.25	117.70
1	AA	451	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	1036	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	282	A	N3-C4-N9	5.10	131.48	127.40
1	AA	1105	A	C5-C6-N1	5.10	120.25	117.70
22	BA	182	A	C4-C5-N7	-5.10	108.15	110.70
23	BB	52	A	N3-C4-N9	5.10	131.48	127.40
1	AA	338	A	N3-C4-N9	5.10	131.48	127.40
1	AA	860	A	N3-C4-N9	5.10	131.48	127.40
1	AA	1431	A	N3-C4-N9	5.10	131.48	127.40
22	BA	2176	A	N3-C4-N9	5.10	131.48	127.40
22	BA	374	A	N3-C4-N9	5.10	131.48	127.40
55	B8	51	A	C4-C5-N7	-5.10	108.15	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	681	A	N3-C4-N9	5.10	131.48	127.40
1	AA	914	A	C8-N9-C4	5.10	107.84	105.80
22	BA	221	A	N3-C4-N9	5.10	131.48	127.40
22	BA	2169	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	2738	A	C4-C5-C6	5.10	119.55	117.00
22	BA	1981	A	C4-C5-C6	5.10	119.55	117.00
1	AA	1493	A	C8-N9-C4	5.10	107.84	105.80
22	BA	402	A	N3-C4-N9	5.10	131.48	127.40
22	BA	1705	A	C5-C6-N1	5.10	120.25	117.70
1	AA	313	A	N3-C4-N9	5.09	131.48	127.40
1	AA	1021	A	N3-C4-N9	5.09	131.48	127.40
1	AA	1513	A	N3-C4-N9	5.09	131.47	127.40
22	BA	644	A	C5-C6-N1	5.09	120.25	117.70
22	BA	2547	A	N3-C4-N9	5.09	131.48	127.40
1	AA	595	A	C4-C5-N7	-5.09	108.15	110.70
22	BA	56	A	C5-C6-N1	5.09	120.25	117.70
1	AA	151	A	C4-C5-C6	5.09	119.55	117.00
22	BA	1098	A	N9-C4-C5	5.09	107.84	105.80
22	BA	1169	A	N3-C4-N9	5.09	131.47	127.40
22	BA	1285	A	C5-C6-N1	5.09	120.25	117.70
22	BA	1528	A	N9-C4-C5	5.09	107.84	105.80
22	BA	1829	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	2411	A	N3-C4-N9	5.09	131.47	127.40
1	AA	81	A	N3-C4-N9	5.09	131.47	127.40
22	BA	1503	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	2636	C	N1-C2-O2	5.09	121.95	118.90
1	AA	452	A	C5-C6-N1	5.09	120.24	117.70
1	AA	831	A	C4-C5-N7	-5.09	108.16	110.70
1	AA	1236	A	N3-C4-N9	5.09	131.47	127.40
1	AA	1261	A	C4-C5-N7	-5.09	108.16	110.70
1	AA	1377	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	38	A	N3-C4-N9	5.09	131.47	127.40
22	BA	646	U	O4'-C1'-N1	5.09	112.27	108.20
22	BA	2740	A	C5-C6-N1	5.09	120.24	117.70
1	AA	1004	A	C4-C5-C6	5.08	119.54	117.00
22	BA	384	A	N3-C4-N9	5.08	131.47	127.40
22	BA	975	A	N3-C4-N9	5.08	131.47	127.40
22	BA	1669	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	1913	A	N3-C4-N9	5.08	131.47	127.40
27	BF	123	ASP	CB-CG-OD1	5.08	122.88	118.30
1	AA	33	A	N9-C4-C5	5.08	107.83	105.80
1	AA	262	A	N3-C4-N9	5.08	131.47	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	749	A	N3-C4-N9	5.08	131.47	127.40
22	BA	300	A	N3-C4-N9	5.08	131.47	127.40
22	BA	990	A	N3-C4-N9	5.08	131.47	127.40
55	B8	73	A	C4-C5-C6	5.08	119.54	117.00
22	BA	2005	A	C4-C5-C6	5.08	119.54	117.00
22	BA	2035	G	O4'-C1'-N9	5.08	112.27	108.20
1	AA	935	A	C5-C6-N1	5.08	120.24	117.70
22	BA	1085	A	N3-C4-N9	5.08	131.46	127.40
22	BA	1264	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	483	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	1331	G	C8-N9-C4	-5.08	104.37	106.40
22	BA	1762	A	C5-C6-N1	5.08	120.24	117.70
22	BA	2738	A	C5-C6-N1	5.08	120.24	117.70
23	BB	115	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	327	A	C5-C6-N1	5.08	120.24	117.70
22	BA	941	A	N3-C4-N9	5.08	131.46	127.40
1	AA	1534	A	C4-C5-N7	-5.07	108.16	110.70
22	BA	401	A	C4-C5-N7	-5.07	108.16	110.70
22	BA	471	A	N3-C4-N9	5.07	131.46	127.40
22	BA	917	A	C4-C5-N7	-5.07	108.16	110.70
22	BA	1754	A	C4-C5-C6	5.07	119.54	117.00
22	BA	2432	A	N3-C4-N9	5.07	131.46	127.40
1	AA	782	A	C4-C5-N7	-5.07	108.16	110.70
22	BA	788	A	N3-C4-N9	5.07	131.46	127.40
22	BA	960	A	N9-C4-C5	5.07	107.83	105.80
1	AA	253	A	N3-C4-N9	5.07	131.46	127.40
1	AA	1333	A	C5-C6-N1	5.07	120.23	117.70
1	AA	1491	G	N3-C4-C5	5.07	131.13	128.60
1	AA	1167	A	C8-N9-C4	5.07	107.83	105.80
22	BA	63	A	N9-C4-C5	5.07	107.83	105.80
22	BA	362	A	N9-C4-C5	5.07	107.83	105.80
22	BA	423	A	N3-C4-N9	5.07	131.45	127.40
22	BA	1100	C	C2-N1-C1'	5.07	124.37	118.80
1	AA	325	A	N3-C4-N9	5.07	131.45	127.40
1	AA	1042	A	N3-C4-N9	5.07	131.45	127.40
22	BA	1204	A	C4-C5-N7	-5.07	108.17	110.70
22	BA	1730	C	C2-N1-C1'	5.07	124.37	118.80
22	BA	547	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	705	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	899	A	N3-C4-N9	5.06	131.45	127.40
1	AA	1105	A	N3-C4-N9	5.06	131.45	127.40
22	BA	896	A	N3-C4-N9	5.06	131.45	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1819	A	C5-C6-N1	5.06	120.23	117.70
1	AA	1374	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	1127	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	1525	A	C8-N9-C4	5.06	107.82	105.80
22	BA	1998	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	2173	A	C4-C5-N7	-5.06	108.17	110.70
23	BB	78	A	N3-C4-N9	5.06	131.45	127.40
1	AA	26	A	C5-C6-N1	5.06	120.23	117.70
1	AA	906	A	N3-C4-N9	5.06	131.44	127.40
1	AA	1429	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	1608	A	C5-C6-N1	5.06	120.23	117.70
22	BA	1847	A	C4-C5-N7	-5.06	108.17	110.70
1	AA	373	A	C4-C5-N7	-5.06	108.17	110.70
1	AA	1476	A	N3-C4-N9	5.05	131.44	127.40
22	BA	10	A	C5-C6-N1	5.05	120.23	117.70
22	BA	1328	A	N3-C4-N9	5.05	131.44	127.40
22	BA	1698	A	N3-C4-N9	5.05	131.44	127.40
22	BA	2205	A	C4-C5-N7	-5.05	108.17	110.70
1	AA	1285	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	21	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	721	A	C5-C6-N1	5.05	120.23	117.70
22	BA	1194	A	N3-C4-N9	5.05	131.44	127.40
1	AA	642	A	N3-C4-N9	5.05	131.44	127.40
1	AA	1044	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	279	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	2660	A	N3-C4-N9	5.05	131.44	127.40
1	AA	98	A	C4-C5-N7	-5.05	108.17	110.70
1	AA	609	A	C4-C5-N7	-5.05	108.17	110.70
1	AA	715	A	C5-C6-N1	5.05	120.22	117.70
1	AA	878	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	1165	A	C4-C5-N7	-5.05	108.18	110.70
22	BA	222	A	C5-C6-N1	5.05	120.22	117.70
1	AA	181	A	N9-C4-C5	5.05	107.82	105.80
1	AA	468	A	N3-C4-N9	5.05	131.44	127.40
1	AA	1468	A	N9-C4-C5	5.05	107.82	105.80
22	BA	44	A	N3-C4-N9	5.05	131.44	127.40
22	BA	2412	A	C4-C5-N7	-5.05	108.18	110.70
22	BA	483	A	N3-C4-N9	5.04	131.44	127.40
1	AA	236	A	C5-C6-N1	5.04	120.22	117.70
1	AA	864	A	C4-C5-N7	-5.04	108.18	110.70
1	AA	1375	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	654	A	C5-C6-N1	5.04	120.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	743	A	C5-C6-N1	5.04	120.22	117.70
22	BA	825	A	N3-C4-N9	5.04	131.44	127.40
22	BA	1351	C	N3-C2-O2	-5.04	118.37	121.90
22	BA	2377	A	N3-C4-N9	5.04	131.44	127.40
22	BA	2531	A	C5-C6-N1	5.04	120.22	117.70
22	BA	2154	A	C5-C6-N1	5.04	120.22	117.70
22	BA	2198	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	1960	A	N3-C4-N9	5.04	131.43	127.40
1	AA	1332	A	N3-C4-N9	5.04	131.43	127.40
22	BA	104	A	N3-C4-N9	5.04	131.43	127.40
22	BA	1143	A	N9-C4-C5	5.04	107.82	105.80
1	AA	766	A	C5-C6-N1	5.04	120.22	117.70
22	BA	2542	A	C5-C6-N1	5.04	120.22	117.70
1	AA	1102	A	C4-C5-N7	-5.04	108.18	110.70
1	AA	1503	A	N3-C4-N9	5.04	131.43	127.40
5	AE	112	ARG	NE-CZ-NH1	5.04	122.82	120.30
22	BA	983	A	C6-N1-C2	5.04	121.62	118.60
22	BA	1434	A	C4-C5-C6	5.04	119.52	117.00
22	BA	1439	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	2171	A	N3-C4-N9	5.04	131.43	127.40
22	BA	42	A	N3-C4-N9	5.03	131.43	127.40
22	BA	1262	A	N3-C4-N9	5.03	131.43	127.40
22	BA	1610	A	C4-C5-N7	-5.03	108.18	110.70
22	BA	1073	A	C4-C5-N7	-5.03	108.18	110.70
1	AA	161	A	N3-C4-N9	5.03	131.42	127.40
22	BA	64	A	C5-C6-N1	5.03	120.22	117.70
22	BA	1384	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	1672	A	C5-C6-N1	5.03	120.22	117.70
22	BA	2835	A	C5-C6-N1	5.03	120.22	117.70
1	AA	1005	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	1365	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	1385	A	C8-N9-C4	5.03	107.81	105.80
1	AA	303	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	181	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	265	A	N3-C4-N9	5.03	131.42	127.40
22	BA	626	A	N3-C4-N9	5.03	131.42	127.40
22	BA	1403	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	1579	A	N3-C4-N9	5.03	131.42	127.40
22	BA	1690	A	N3-C4-N9	5.03	131.42	127.40
22	BA	2388	A	N3-C4-N9	5.03	131.42	127.40
1	AA	495	A	C8-N9-C4	5.03	107.81	105.80
1	AA	716	A	N3-C4-N9	5.03	131.42	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	915	A	C5-C6-N1	5.03	120.21	117.70
1	AA	974	A	C4-C5-N7	-5.03	108.19	110.70
1	AA	1350	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	101	A	N9-C4-C5	5.03	107.81	105.80
22	BA	1046	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	1815	A	N3-C4-N9	5.03	131.42	127.40
22	BA	825	A	C5-C6-N1	5.02	120.21	117.70
1	AA	190	A	N9-C4-C5	5.02	107.81	105.80
1	AA	560	A	N3-C4-N9	5.02	131.42	127.40
22	BA	195	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	2781	A	N3-C4-N9	5.02	131.42	127.40
1	AA	869	G	C5-C6-O6	5.02	131.61	128.60
22	BA	1392	A	N3-C4-N9	5.02	131.42	127.40
55	B8	41	A	N9-C4-C5	5.02	107.81	105.80
1	AA	1229	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	1525	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	1717	A	N3-C4-N9	5.02	131.41	127.40
22	BA	2158	A	N3-C4-N9	5.02	131.41	127.40
1	AA	1339	A	N3-C4-N9	5.02	131.41	127.40
22	BA	2501	C	C2-N1-C1'	-5.02	113.28	118.80
1	AA	878	A	N3-C4-N9	5.02	131.41	127.40
22	BA	142	A	C4-C5-N7	-5.02	108.19	110.70
1	AA	1257	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	1289	C	C6-N1-C2	-5.01	118.29	120.30
22	BA	1307	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	2163	A	C4-C5-N7	-5.01	108.19	110.70
23	BB	73	A	N9-C4-C5	5.01	107.81	105.80
1	AA	51	A	N3-C4-N9	5.01	131.41	127.40
22	BA	19	A	C8-N9-C4	5.01	107.81	105.80
22	BA	2183	A	N3-C4-N9	5.01	131.41	127.40
22	BA	2330	G	C8-N9-C4	-5.01	104.39	106.40
1	AA	353	A	N3-C4-N9	5.01	131.41	127.40
1	AA	364	A	C4-C5-N7	-5.01	108.19	110.70
1	AA	470	C	N3-C2-O2	-5.01	118.39	121.90
1	AA	994	A	C4-C5-N7	-5.01	108.19	110.70
1	AA	1169	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	1801	A	N3-C4-N9	5.01	131.41	127.40
22	BA	2059	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	2108	A	N3-C4-N9	5.01	131.41	127.40
22	BA	2327	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	2482	A	N9-C4-C5	5.01	107.80	105.80
22	BA	2727	A	C5-C6-N1	5.01	120.20	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BB	115	A	C5-C6-N1	5.01	120.21	117.70
1	AA	320	A	C5-C6-N1	5.01	120.20	117.70
1	AA	831	A	N3-C4-N9	5.01	131.41	127.40
22	BA	1490	A	C4-C5-N7	-5.01	108.20	110.70
23	BB	78	A	C5-C6-N1	5.01	120.20	117.70
1	AA	1167	A	N3-C4-N9	5.01	131.41	127.40
22	BA	1086	A	C4-C5-N7	-5.01	108.20	110.70
22	BA	2311	A	N3-C4-N9	5.01	131.41	127.40
22	BA	42	A	C5-C6-N1	5.01	120.20	117.70
22	BA	1735	A	N3-C4-N9	5.01	131.41	127.40
22	BA	2161	C	N3-C2-O2	-5.00	118.40	121.90
1	AA	26	A	C4-C5-C6	5.00	119.50	117.00
1	AA	968	A	C4-C5-N7	-5.00	108.20	110.70
1	AA	1394	A	N3-C4-N9	5.00	131.40	127.40
22	BA	13	A	N3-C4-N9	5.00	131.40	127.40
22	BA	429	A	N3-C4-N9	5.00	131.40	127.40
22	BA	513	A	N9-C4-C5	5.00	107.80	105.80
22	BA	1342	A	C4-C5-C6	5.00	119.50	117.00
22	BA	1496	A	C5-C6-N1	5.00	120.20	117.70
22	BA	1598	A	C5-C6-N1	5.00	120.20	117.70
1	AA	172	A	C4-C5-N7	-5.00	108.20	110.70
22	BA	632	A	N3-C4-N9	5.00	131.40	127.40
22	BA	1877	A	C4-C5-N7	-5.00	108.20	110.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	204	ASP	Sidechain
2	AB	205	ASP	Sidechain
7	AG	24	ALA	Mainchain
29	BH	104	THR	Peptide
29	BH	66	ASN	Peptide
43	BV	34	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16580	240	0
2	AB	1753	0	1780	60	0
3	AC	1624	0	1696	41	0
4	AD	1643	0	1707	38	0
5	AE	1144	0	1185	25	0
6	AF	862	0	864	34	0
7	AG	1181	0	1238	31	0
8	AH	979	0	1031	29	0
9	AI	1022	0	1070	36	0
10	AJ	795	0	836	26	0
11	AK	877	0	887	16	0
12	AL	957	0	1017	12	0
13	AM	883	0	941	25	0
14	AN	799	0	841	23	0
15	AO	714	0	734	18	0
16	AP	649	0	666	10	0
17	AQ	648	0	691	12	0
18	AR	455	0	478	13	0
19	AS	656	0	680	25	0
20	AT	670	0	719	10	0
21	AU	465	0	491	9	0
22	BA	62209	0	31290	320	0
23	BB	2569	0	1301	7	0
24	BC	2082	0	2154	27	0
25	BD	1566	0	1617	12	0
26	BE	1552	0	1619	10	0
27	BF	1410	0	1444	26	0
28	BG	1323	0	1371	18	0
29	BH	1110	0	1148	28	0
30	BI	522	0	520	13	0
31	BJ	1129	0	1162	14	0
32	BK	946	0	1023	13	0
33	BL	1053	0	1128	12	0
34	BM	1075	0	1155	14	0
35	BN	945	0	989	9	0
36	BO	900	0	935	8	0
37	BP	917	0	962	9	0
38	BQ	947	0	1019	7	0
39	BR	816	0	839	7	0
40	BS	857	0	922	7	0
41	BT	738	0	807	10	0
42	BU	779	0	831	11	0
43	BV	753	0	780	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BW	580	0	594	21	0
45	BX	625	0	652	4	0
46	BY	501	0	531	5	0
47	BZ	449	0	488	1	0
48	B0	444	0	458	5	0
49	B1	414	0	442	12	0
50	B2	377	0	418	5	0
51	B3	504	0	572	4	0
52	B4	302	0	340	4	0
53	B5	146	0	139	3	0
54	B7	191	0	99	0	0
55	B8	1648	0	833	27	0
56	AA	86	0	0	0	0
56	B8	2	0	0	0	0
56	BA	233	0	0	0	0
56	BB	1	0	0	0	0
56	BC	1	0	0	0	0
56	BD	2	0	0	0	0
56	BL	1	0	0	0	0
57	AA	38	0	0	0	0
57	AM	1	0	0	0	0
57	BA	104	0	0	1	0
57	BB	1	0	0	0	0
57	BC	1	0	0	0	0
57	BD	1	0	0	0	0
57	BM	1	0	0	0	0
58	AB	1	0	0	0	0
58	B4	1	0	0	0	0
58	BI	1	0	0	0	0
59	BA	15	0	9	0	0
60	AA	184	0	0	1	0
60	AK	1	0	0	0	0
60	AN	1	0	0	0	0
60	B0	4	0	0	0	0
60	B2	6	0	0	0	0
60	B3	7	0	0	0	0
60	B4	1	0	0	0	0
60	B5	2	0	0	1	0
60	B8	3	0	0	1	0
60	BA	1672	0	0	25	0
60	BB	2	0	0	0	0
60	BC	38	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BD	14	0	0	0	0
60	BE	21	0	0	2	0
60	BF	1	0	0	0	0
60	BJ	2	0	0	0	0
60	BK	3	0	0	0	0
60	BL	14	0	0	0	0
60	BM	2	0	0	0	0
60	BN	9	0	0	0	0
60	BO	1	0	0	0	0
60	BP	2	0	0	0	0
60	BQ	12	0	0	0	0
60	BR	4	0	0	0	0
60	BS	7	0	0	0	0
60	BT	3	0	0	0	0
60	BU	1	0	0	0	0
60	BW	5	0	0	3	0
60	BX	4	0	0	0	0
All	All	146602	0	96723	1260	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 5.

All (1260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:39:LEU:HD11	6:AF:62:MET:CE	1.55	1.34
6:AF:39:LEU:CD1	6:AF:62:MET:CE	2.07	1.33
42:BU:10:GLU:OE2	42:BU:73:PHE:HB3	1.34	1.23
6:AF:39:LEU:CD1	6:AF:62:MET:HE2	1.65	1.19
6:AF:39:LEU:HD12	6:AF:62:MET:HG2	1.27	1.14
55:B8:22:G:N7	55:B8:46:G7M:N2	1.96	1.13
49:B1:35:GLU:OE1	49:B1:48:ILE:HG23	1.49	1.12
14:AN:49:GLN:NE2	19:AS:10:PHE:CE1	2.22	1.08
22:BA:2330:G:O2'	44:BW:44:LYS:NZ	1.87	1.06
44:BW:42:GLY:H	44:BW:44:LYS:HZ3	1.04	1.03
6:AF:39:LEU:HD11	6:AF:62:MET:HE3	1.36	1.02
42:BU:10:GLU:OE2	42:BU:73:PHE:CB	2.09	1.00
6:AF:39:LEU:HD11	6:AF:62:MET:HE2	1.18	1.00
6:AF:39:LEU:HD12	6:AF:62:MET:CG	1.91	0.99
27:BF:94:GLU:OE2	27:BF:98:GLU:OE2	1.79	0.99
7:AG:74:GLU:HG2	7:AG:91:VAL:HG22	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:74:GLU:HG2	7:AG:91:VAL:CG2	1.94	0.98
5:AE:83:HIS:NE2	5:AE:147:MET:HG3	1.85	0.92
1:AA:49:U:C4	1:AA:365:U:O4	2.23	0.92
6:AF:39:LEU:CD1	6:AF:62:MET:HG2	2.00	0.92
14:AN:49:GLN:HE21	19:AS:10:PHE:HE1	1.18	0.91
14:AN:49:GLN:NE2	19:AS:10:PHE:CZ	2.39	0.90
6:AF:39:LEU:HD13	6:AF:62:MET:HE2	1.51	0.90
1:AA:49:U:O4	1:AA:365:U:O4	1.91	0.88
1:AA:49:U:C5	1:AA:365:U:O4	2.28	0.87
17:AQ:77:ARG:HE	17:AQ:79:VAL:HG12	1.40	0.86
49:B1:35:GLU:OE1	49:B1:48:ILE:CG2	2.23	0.86
28:BG:24:ILE:HD11	28:BG:43:VAL:HG11	1.59	0.84
6:AF:101:PRO:HG2	18:AR:25:ASP:OD1	1.77	0.84
6:AF:39:LEU:HD13	6:AF:62:MET:CE	2.03	0.83
44:BW:41:ARG:H	44:BW:44:LYS:HE2	1.43	0.82
25:BD:184:ARG:NH1	37:BP:7:GLN:OE1	2.14	0.81
3:AC:132:ARG:HG2	3:AC:136:ARG:NH1	1.95	0.81
5:AE:94:VAL:HG13	5:AE:111:MET:HE3	1.61	0.81
44:BW:44:LYS:HD2	44:BW:44:LYS:H	1.45	0.81
2:AB:15:HIS:HB3	2:AB:43:LEU:HD21	1.61	0.81
3:AC:135:LYS:O	3:AC:139:GLN:HG2	1.81	0.80
5:AE:112:ARG:HG3	5:AE:112:ARG:HH11	1.46	0.80
2:AB:165:ASP:HB2	2:AB:204:ASP:OD1	1.81	0.80
55:B8:18:G:O2'	55:B8:57:G:N2	2.15	0.80
6:AF:22:ILE:HG23	6:AF:62:MET:CE	2.13	0.79
29:BH:81:ALA:HB1	29:BH:149:GLU:HG2	1.63	0.79
2:AB:6:MET:SD	2:AB:47:VAL:HG11	2.23	0.79
42:BU:8:ASP:OD1	42:BU:24:LYS:NZ	2.15	0.78
9:AI:28:ILE:HG12	9:AI:63:LEU:HD21	1.66	0.78
11:AK:53:ARG:HH12	11:AK:57:LYS:HD3	1.46	0.78
8:AH:95:VAL:O	8:AH:96:MET:HB3	1.84	0.78
7:AG:50:LEU:HD21	7:AG:124:LEU:HB3	1.64	0.78
3:AC:84:VAL:HG23	3:AC:88:ARG:NH1	1.99	0.77
3:AC:132:ARG:HG2	3:AC:136:ARG:HH12	1.48	0.77
6:AF:39:LEU:CD1	6:AF:62:MET:CG	2.59	0.77
1:AA:401:C:OP2	4:AD:70:ARG:NH1	2.16	0.76
22:BA:2189:U:H2'	22:BA:2190:G:C8	2.21	0.76
29:BH:82:SER:N	29:BH:149:GLU:HG3	2.01	0.76
22:BA:2840:C:H5"	35:BN:53:THR:HG21	1.67	0.75
6:AF:38:ARG:HH21	6:AF:61:LEU:HD21	1.51	0.75
22:BA:760:G:OP1	60:BA:3402:HOH:O	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:74:GLU:CG	7:AG:91:VAL:HG22	2.16	0.75
6:AF:39:LEU:CD1	6:AF:62:MET:SD	2.74	0.75
22:BA:1800:C:OP2	24:BC:182:ARG:NH2	2.20	0.75
11:AK:23:ILE:HG12	11:AK:96:THR:HG21	1.66	0.74
11:AK:64:GLN:HG3	11:AK:99:ALA:HB2	1.68	0.74
10:AJ:22:THR:HG21	10:AJ:72:ARG:HG2	1.70	0.74
9:AI:18:ARG:HG2	9:AI:66:THR:HG22	1.69	0.74
55:B8:55:PSU:O2'	55:B8:57:G:N7	2.20	0.74
6:AF:22:ILE:HG23	6:AF:62:MET:HE2	1.70	0.74
6:AF:39:LEU:HD13	6:AF:62:MET:SD	2.28	0.74
22:BA:1649:G:O2'	35:BN:106:ASP:OD2	2.06	0.74
6:AF:39:LEU:CD1	6:AF:62:MET:HE3	2.01	0.73
1:AA:742:G:OP1	15:AO:58:ARG:NH2	2.21	0.73
4:AD:56:ARG:HE	4:AD:56:ARG:HA	1.53	0.73
60:BA:3713:HOH:O	38:BQ:41:LYS:HE3	1.88	0.73
1:AA:458:U:H2'	1:AA:459:A:C8	2.22	0.73
1:AA:458:U:H2'	1:AA:459:A:H8	1.52	0.73
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.23	0.73
24:BC:148:PRO:CD	24:BC:185:GLU:OE2	2.36	0.73
15:AO:89:ARG:NH2	22:BA:714:U:O4	2.22	0.73
13:AM:16:VAL:HB	13:AM:41:GLU:HB2	1.71	0.72
22:BA:2131:U:H5'	22:BA:2132:U:H5"	1.71	0.72
22:BA:2134:A:OP2	22:BA:2157:G:N2	2.22	0.72
18:AR:26:ILE:HD11	18:AR:67:LEU:HD22	1.71	0.72
7:AG:67:GLU:OE2	7:AG:70:ARG:NH2	2.22	0.72
57:BA:3260:K:K	60:BA:3487:HOH:O	2.00	0.72
22:BA:1047:G:HO2'	22:BA:1110:G:H1	1.35	0.72
22:BA:2898:U:O2'	31:BJ:136:GLN:NE2	2.23	0.71
8:AH:43:GLU:HG2	8:AH:101:ILE:HG21	1.71	0.71
9:AI:106:ARG:NH1	9:AI:107:ASP:O	2.23	0.71
3:AC:84:VAL:O	3:AC:88:ARG:HG2	1.89	0.71
26:BE:164:LEU:O	60:BE:301:HOH:O	2.07	0.71
22:BA:1155:A:OP2	60:BA:3403:HOH:O	2.09	0.71
22:BA:2470:G:OP1	34:BM:55:ARG:NH2	2.23	0.71
49:B1:5:ILE:HD12	49:B1:28:ARG:HH21	1.54	0.71
1:AA:1151:A:H5"	10:AJ:44:THR:HG23	1.71	0.71
1:AA:1061:G:OP2	3:AC:3:GLN:NE2	2.24	0.71
19:AS:67:VAL:O	30:BI:56:ARG:NH2	2.24	0.71
55:B8:12:G:OP2	60:B8:201:HOH:O	2.08	0.70
22:BA:1250:G:H5"	38:BQ:6:ARG:HD3	1.72	0.70
1:AA:544:G:OP1	4:AD:56:ARG:NH2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:50:LEU:HD11	7:AG:121:ALA:HA	1.73	0.70
1:AA:823:C:HO2'	8:AH:2:SER:N	1.89	0.70
44:BW:39:ARG:HD3	60:BW:104:HOH:O	1.90	0.70
44:BW:40:GLN:HB2	44:BW:44:LYS:HE2	1.73	0.70
10:AJ:6:ILE:HG22	10:AJ:76:ILE:HB	1.73	0.70
40:BS:59:GLU:OE2	40:BS:66:ILE:HB	1.92	0.70
1:AA:1055:A:O2'	3:AC:156:ARG:NH1	2.25	0.69
22:BA:666:A:O2'	60:BA:3404:HOH:O	2.10	0.69
1:AA:600:A:H5"	8:AH:89:LYS:HD2	1.75	0.69
2:AB:18:HIS:NE2	2:AB:205:ASP:OD2	2.26	0.69
30:BI:14:ALA:HB1	30:BI:34:LEU:HD21	1.75	0.69
2:AB:122:GLN:O	2:AB:125:THR:OG1	2.10	0.69
3:AC:151:VAL:HG22	3:AC:200:VAL:HG22	1.74	0.69
9:AI:12:ARG:NH1	9:AI:107:ASP:OD2	2.25	0.68
44:BW:42:GLY:H	44:BW:44:LYS:NZ	1.86	0.68
4:AD:12:SER:OG	4:AD:17:THR:O	2.11	0.68
25:BD:16:THR:HG22	25:BD:18:ASP:H	1.59	0.68
1:AA:600:A:H5"	8:AH:89:LYS:CD	2.24	0.68
3:AC:142:MET:HG3	3:AC:170:GLU:HG2	1.76	0.67
22:BA:1607:C:OP2	60:BA:3405:HOH:O	2.12	0.67
22:BA:2185:U:H2'	22:BA:2186:G:C8	2.29	0.67
4:AD:100:ASN:OD1	4:AD:111:ARG:NH1	2.28	0.67
22:BA:140:C:H5'	22:BA:141:G:N7	2.09	0.67
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	1.94	0.67
13:AM:17:ILE:O	13:AM:20:THR:OG1	2.11	0.67
22:BA:882:G:N2	22:BA:883:G:N7	2.42	0.67
2:AB:18:HIS:HE2	2:AB:188:ASP:CG	1.98	0.67
10:AJ:40:ILE:HG22	10:AJ:73:LEU:HB3	1.77	0.66
29:BH:9:VAL:HG23	29:BH:12:LEU:HB2	1.76	0.66
14:AN:9:GLU:O	14:AN:13:VAL:HG23	1.96	0.66
6:AF:66:ALA:HB3	6:AF:71:ILE:HD11	1.76	0.66
2:AB:6:MET:HE3	2:AB:43:LEU:HB3	1.78	0.66
1:AA:382:A:H2'	1:AA:383:A:C8	2.31	0.66
1:AA:1059:C:O3'	14:AN:85:ARG:NH2	2.29	0.66
1:AA:1147:C:O2	9:AI:18:ARG:NH1	2.29	0.66
22:BA:286:U:H2'	22:BA:287:G:H8	1.61	0.66
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.31	0.66
5:AE:112:ARG:HG3	5:AE:112:ARG:NH1	2.08	0.65
14:AN:16:ALA:HA	14:AN:55:SER:HA	1.77	0.65
22:BA:2033:A:OP1	60:BA:3406:HOH:O	2.15	0.65
48:B0:55:ILE:HD12	48:B0:57:LYS:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1225:A:H3'	13:AM:102:THR:HG21	1.79	0.65
4:AD:57:GLU:HG2	4:AD:199:LEU:HD12	1.79	0.65
1:AA:1505:G:OP2	60:AA:1802:HOH:O	0.65	0.65
6:AF:86:ARG:NH1	18:AR:64:TYR:O	2.29	0.65
32:BK:66:LYS:HE2	32:BK:81:GLY:HA2	1.77	0.65
1:AA:1320:C:H5"	19:AS:3:ARG:HH12	1.62	0.64
1:AA:1356:G:H2'	1:AA:1357:A:H8	1.60	0.64
22:BA:248:G:N3	60:BA:3434:HOH:O	2.30	0.64
53:B5:17:ASN:ND2	60:B5:101:HOH:O	2.30	0.64
9:AI:47:VAL:CG2	9:AI:76:ALA:HB1	2.28	0.64
22:BA:1797:G:HO2'	24:BC:257:THR:HG1	1.44	0.64
5:AE:80:THR:OG1	5:AE:122:ASN:O	2.14	0.64
7:AG:74:GLU:HG2	7:AG:91:VAL:HG21	1.77	0.64
21:AU:28:VAL:HA	21:AU:31:GLU:HB2	1.79	0.64
42:BU:10:GLU:OE1	42:BU:22:ARG:HD2	1.97	0.64
28:BG:42:GLU:HB3	28:BG:55:ARG:HH21	1.62	0.64
22:BA:568:U:H1'	22:BA:2030:6MZ:H9C1	1.79	0.64
1:AA:49:U:O4	1:AA:365:U:C4	2.51	0.64
49:B1:7:GLU:OE1	49:B1:9:ILE:HG23	1.98	0.64
1:AA:346:G:OP1	37:BP:39:ARG:NH1	2.28	0.63
6:AF:99:ALA:O	6:AF:104:LYS:NZ	2.31	0.63
22:BA:651:G:H5'	51:B3:19:LYS:HG3	1.81	0.63
41:BT:92:ASN:O	41:BT:93:LEU:HB2	1.97	0.63
3:AC:84:VAL:HG23	3:AC:88:ARG:HH12	1.61	0.63
22:BA:1434:A:H2'	22:BA:1435:G:C8	2.33	0.63
22:BA:2327:A:H2'	22:BA:2328:A:C8	2.33	0.63
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.80	0.63
5:AE:83:HIS:CE1	5:AE:85:VAL:HG12	2.33	0.63
38:BQ:89:GLU:O	38:BQ:89:GLU:HG2	1.98	0.63
2:AB:47:VAL:HG23	2:AB:48:PRO:HD3	1.81	0.63
3:AC:76:VAL:HG23	3:AC:103:ILE:HD13	1.79	0.63
46:BY:27:ASN:O	46:BY:31:GLN:HG3	1.99	0.63
4:AD:65:TYR:CE2	4:AD:94:LEU:HB3	2.34	0.62
10:AJ:8:ILE:HD12	10:AJ:74:VAL:HG13	1.80	0.62
22:BA:536:G:OP2	60:BA:3407:HOH:O	2.16	0.62
22:BA:1469:A:H2'	22:BA:1470:A:C8	2.33	0.62
27:BF:10:ASP:O	27:BF:14:LYS:NZ	2.29	0.62
10:AJ:18:ILE:O	10:AJ:22:THR:HG23	1.99	0.62
22:BA:2188:U:H2'	22:BA:2189:U:C6	2.34	0.62
31:BJ:13:ARG:NH2	31:BJ:49:ASP:O	2.32	0.62
33:BL:69:ARG:HG2	33:BL:69:ARG:HH11	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AT:44:LYS:HG3	20:AT:87:ALA:HB3	1.81	0.62
28:BG:32:GLU:OE2	28:BG:34:THR:OG1	2.17	0.62
22:BA:1434:A:H2'	22:BA:1435:G:H8	1.64	0.62
1:AA:1103:C:OP1	2:AB:95:ARG:NH2	2.32	0.62
1:AA:1339:A:H2	55:B8:30:C:HO2'	1.46	0.62
27:BF:103:LEU:O	27:BF:108:VAL:HG13	2.00	0.62
6:AF:45:ARG:O	6:AF:56:LYS:HA	1.98	0.61
9:AI:47:VAL:HG21	9:AI:76:ALA:HB1	1.82	0.61
15:AO:55:GLY:O	15:AO:59:MET:HG3	2.00	0.61
1:AA:673:A:H2'	1:AA:674:G:C8	2.35	0.61
17:AQ:77:ARG:HE	17:AQ:79:VAL:CG1	2.10	0.61
22:BA:2159:G:H2'	22:BA:2160:C:C6	2.36	0.61
11:AK:84:VAL:HG11	11:AK:97:ILE:HD11	1.81	0.61
12:AL:51:LYS:HD2	12:AL:51:LYS:N	2.16	0.61
14:AN:80:SER:O	14:AN:84:VAL:HG12	1.99	0.61
22:BA:992:C:OP1	39:BR:76:LYS:NZ	2.34	0.61
22:BA:2250:G:OP1	34:BM:84:LYS:NZ	2.32	0.61
30:BI:35:ASP:OD1	30:BI:35:ASP:N	2.34	0.61
3:AC:22:TRP:HB3	3:AC:59:ARG:HB2	1.81	0.61
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.36	0.61
28:BG:170:ARG:NH1	52:B4:29:ALA:O	2.33	0.61
44:BW:44:LYS:H	44:BW:44:LYS:CD	2.14	0.61
10:AJ:10:LEU:HD12	10:AJ:22:THR:HG22	1.82	0.61
28:BG:117:LEU:HD13	28:BG:118:PRO:HD2	1.83	0.61
22:BA:2187:U:H2'	22:BA:2188:U:O4'	2.01	0.61
27:BF:118:SER:OG	27:BF:120:LYS:HG2	2.00	0.60
28:BG:4:VAL:O	28:BG:69:ARG:HD2	2.01	0.60
49:B1:33:LYS:HD3	49:B1:51:GLU:HB3	1.83	0.60
23:BB:75:G:HO2'	43:BV:88:HIS:HE2	1.47	0.60
26:BE:80:SER:OG	60:BE:302:HOH:O	2.13	0.60
22:BA:2273:A:H2'	22:BA:2274:A:C8	2.37	0.60
22:BA:2032:G:C5	25:BD:150:MEQ:HE3	2.37	0.60
22:BA:2176:A:H2'	22:BA:2177:C:C6	2.37	0.60
3:AC:53:SER:HB3	3:AC:115:LEU:HD21	1.83	0.60
19:AS:65:GLU:O	30:BI:56:ARG:NH1	2.34	0.60
22:BA:275:C:H2'	22:BA:276:U:H4'	1.83	0.60
22:BA:2189:U:H2'	22:BA:2190:G:H8	1.61	0.60
42:BU:10:GLU:OE2	42:BU:73:PHE:CD2	2.55	0.60
49:B1:37:LYS:NZ	49:B1:46:HIS:O	2.25	0.60
1:AA:337:G:H2'	1:AA:338:A:C8	2.36	0.60
2:AB:133:GLU:HB3	2:AB:137:ARG:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:38:ARG:HG2	6:AF:63:ASN:HB3	1.84	0.60
8:AH:106:THR:HG22	8:AH:107:SER:N	2.15	0.60
2:AB:6:MET:SD	2:AB:47:VAL:CG1	2.89	0.60
1:AA:684:U:O4'	11:AK:40:ASN:ND2	2.35	0.59
7:AG:4:ARG:HG3	7:AG:4:ARG:HH11	1.67	0.59
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.35	0.59
1:AA:746:A:H2'	1:AA:747:A:C8	2.37	0.59
7:AG:149:LYS:HG2	11:AK:61:PHE:CE2	2.37	0.59
1:AA:613:C:OP1	4:AD:81:ARG:NH1	2.29	0.59
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.83	0.59
22:BA:1970:A:H5"	22:BA:1971:U:OP1	2.02	0.59
22:BA:2068:U:N3	22:BA:2430:A:C2	2.71	0.59
32:BK:105:ARG:HG2	32:BK:108:ARG:HD2	1.84	0.59
22:BA:2184:A:H2'	22:BA:2185:U:C6	2.37	0.59
43:BV:75:GLN:HB2	43:BV:92:VAL:HG23	1.83	0.59
9:AI:88:MET:HE3	9:AI:92:GLU:HA	1.84	0.59
44:BW:42:GLY:N	44:BW:44:LYS:HZ3	1.88	0.59
60:BA:4942:HOH:O	38:BQ:11:ARG:HD2	2.03	0.59
24:BC:148:PRO:CG	24:BC:185:GLU:OE2	2.51	0.59
35:BN:72:ASP:OD2	35:BN:75:ILE:HG12	2.03	0.59
4:AD:105:MET:SD	4:AD:180:GLY:HA3	2.43	0.59
5:AE:157:ARG:NH2	8:AH:99:LEU:O	2.36	0.59
8:AH:30:SER:O	8:AH:34:VAL:HG23	2.01	0.59
8:AH:106:THR:HG21	8:AH:121:LEU:HB3	1.85	0.59
6:AF:101:PRO:CG	18:AR:25:ASP:OD1	2.48	0.59
22:BA:281:C:H2'	22:BA:282:A:H8	1.68	0.59
22:BA:639:U:H2'	22:BA:640:C:C6	2.38	0.59
22:BA:1386:C:OP1	60:BA:3408:HOH:O	2.17	0.59
22:BA:2134:A:N6	22:BA:2157:G:O2'	2.36	0.59
24:BC:148:PRO:HD3	24:BC:185:GLU:OE2	2.02	0.59
41:BT:33:LYS:HG2	41:BT:80:TRP:CZ3	2.38	0.59
44:BW:44:LYS:HD2	44:BW:44:LYS:N	2.16	0.59
10:AJ:48:ARG:NH1	10:AJ:66:GLU:OE1	2.36	0.58
22:BA:832:U:H2'	22:BA:833:A:C8	2.38	0.58
22:BA:2107:G:H2'	22:BA:2108:A:C8	2.38	0.58
28:BG:117:LEU:HD12	28:BG:121:ILE:HB	1.84	0.58
3:AC:127:ARG:NH1	3:AC:127:ARG:HB2	2.18	0.58
22:BA:1007:C:OP1	31:BJ:37:ARG:NH1	2.37	0.58
6:AF:22:ILE:HG23	6:AF:62:MET:HE1	1.86	0.58
25:BD:35:THR:HG22	25:BD:73:VAL:HG21	1.85	0.58
27:BF:140:GLU:HA	30:BI:28:VAL:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:15:LEU:HD22	29:BH:15:LEU:H	1.67	0.58
11:AK:97:ILE:HG22	21:AU:12:PHE:CZ	2.38	0.58
1:AA:539:A:H2'	1:AA:540:G:C8	2.38	0.58
22:BA:250:G:H2'	22:BA:251:A:C8	2.38	0.58
22:BA:414:C:H2'	22:BA:415:A:C8	2.37	0.58
28:BG:2:SER:OG	28:BG:3:ARG:N	2.30	0.58
29:BH:108:VAL:HG13	29:BH:109:GLU:H	1.69	0.58
44:BW:41:ARG:N	44:BW:44:LYS:HE2	2.16	0.58
17:AQ:20:SER:HB3	17:AQ:71:LYS:HZ2	1.69	0.58
30:BI:43:PHE:HA	30:BI:46:GLY:HA3	1.84	0.58
22:BA:871:U:H2'	22:BA:872:U:C6	2.37	0.58
1:AA:445:G:H1	1:AA:489:C:H5	1.51	0.58
60:BA:4826:HOH:O	50:B2:46:LYS:HD3	2.02	0.58
4:AD:160:GLU:O	4:AD:164:GLN:HG2	2.03	0.57
17:AQ:39:LYS:HZ3	17:AQ:39:LYS:C	2.07	0.57
22:BA:286:U:H2'	22:BA:287:G:C8	2.37	0.57
60:BA:3605:HOH:O	24:BC:227:PRO:HD2	2.04	0.57
42:BU:10:GLU:OE2	42:BU:73:PHE:CG	2.56	0.57
11:AK:53:ARG:NH1	11:AK:57:LYS:HD3	2.16	0.57
14:AN:15:LEU:O	14:AN:18:LYS:HB3	2.04	0.57
22:BA:2328:A:H2'	22:BA:2329:U:C6	2.39	0.57
2:AB:111:ILE:HG22	2:AB:148:LEU:HD13	1.86	0.57
22:BA:1869:G:N2	22:BA:1871:A:O2'	2.38	0.57
30:BI:30:HIS:CG	30:BI:31:ASP:H	2.21	0.57
7:AG:26:PHE:CD1	7:AG:101:MET:HG2	2.40	0.57
31:BJ:69:ARG:HG2	31:BJ:90:GLU:HG3	1.86	0.57
2:AB:18:HIS:NE2	2:AB:188:ASP:CG	2.58	0.57
3:AC:127:ARG:HB2	3:AC:127:ARG:HH11	1.68	0.57
8:AH:106:THR:HG21	8:AH:121:LEU:CB	2.34	0.57
1:AA:1038:C:H2'	1:AA:1039:G:H8	1.67	0.57
42:BU:10:GLU:OE1	42:BU:22:ARG:HB3	2.04	0.57
1:AA:1320:C:OP2	19:AS:3:ARG:NH1	2.38	0.57
10:AJ:84:VAL:HG13	10:AJ:85:ASP:H	1.69	0.57
10:AJ:84:VAL:O	10:AJ:88:MET:HG3	2.04	0.57
15:AO:58:ARG:CZ	15:AO:58:ARG:HB3	2.34	0.57
1:AA:375:U:H4'	16:AP:17:TYR:CE2	2.40	0.57
22:BA:254:G:N7	51:B3:5:LYS:NZ	2.53	0.57
1:AA:1287:A:H2'	1:AA:1288:A:C8	2.40	0.57
7:AG:27:VAL:HG12	7:AG:43:VAL:HG21	1.87	0.57
55:B8:22:G:N7	55:B8:46:G7M:C2	2.67	0.57
1:AA:216:U:H2'	1:AA:217:C:C6	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:492:C:H2'	1:AA:493:A:C8	2.40	0.56
13:AM:64:VAL:HG11	13:AM:72:GLU:OE2	2.04	0.56
15:AO:78:TYR:O	15:AO:82:ILE:HG23	2.05	0.56
22:BA:2636:C:O2'	25:BD:45:TYR:OH	2.19	0.56
20:AT:66:LEU:HD23	20:AT:67:ILE:HG23	1.87	0.56
22:BA:1177:G:H2'	22:BA:1178:C:H6	1.70	0.56
29:BH:104:THR:HA	29:BH:107:GLY:N	2.20	0.56
44:BW:40:GLN:HB2	44:BW:44:LYS:HD3	1.87	0.56
10:AJ:63:ASP:OD1	14:AN:98:LYS:NZ	2.39	0.56
22:BA:910:A:H2'	22:BA:911:A:C8	2.40	0.56
22:BA:2753:A:O2'	52:B4:15:LYS:HE3	2.04	0.56
29:BH:8:LYS:HD3	29:BH:14:SER:HB3	1.86	0.56
2:AB:97:LEU:HB2	2:AB:100:MET:SD	2.45	0.56
2:AB:70:VAL:HG12	2:AB:163:VAL:HA	1.86	0.56
12:AL:94:ARG:HG3	12:AL:94:ARG:HH11	1.71	0.56
3:AC:42:TYR:HD1	3:AC:43:LEU:HD12	1.69	0.56
1:AA:363:A:OP2	12:AL:31:ARG:NH2	2.35	0.56
22:BA:682:G:H5'	50:B2:26:ASN:OD1	2.06	0.56
29:BH:104:THR:HG21	29:BH:110:VAL:N	2.21	0.56
42:BU:15:THR:HB	42:BU:69:ASN:ND2	2.21	0.56
1:AA:1040:U:H2'	1:AA:1041:G:H8	1.70	0.56
9:AI:43:THR:O	9:AI:47:VAL:HG13	2.06	0.56
24:BC:5:LYS:NZ	24:BC:16:VAL:O	2.39	0.56
49:B1:27:LYS:HA	49:B1:27:LYS:HE2	1.87	0.56
22:BA:249:C:O2	51:B3:12:LYS:NZ	2.39	0.56
55:B8:2:G:O2'	55:B8:3:G:H2'	2.06	0.56
1:AA:299:G:H2'	1:AA:300:A:C8	2.41	0.55
1:AA:1320:C:O2	19:AS:36:ARG:NH2	2.39	0.55
2:AB:163:VAL:N	2:AB:184:PHE:O	2.30	0.55
1:AA:1250:A:H2'	1:AA:1251:A:C8	2.41	0.55
1:AA:944:G:N1	1:AA:1338:G:OP2	2.34	0.55
22:BA:2469:A:N6	22:BA:2481:G:O2'	2.40	0.55
24:BC:267:ILE:HD13	24:BC:270:ARG:HH21	1.70	0.55
7:AG:93:PRO:HA	7:AG:96:ARG:HG3	1.88	0.55
22:BA:526:A:H2'	60:BA:4631:HOH:O	2.06	0.55
22:BA:856:G:H2'	22:BA:857:G:C8	2.41	0.55
10:AJ:57:VAL:O	10:AJ:57:VAL:HG13	2.06	0.55
55:B8:3:G:H4'	55:B8:4:U:OP1	2.07	0.55
3:AC:117:ALA:O	3:AC:121:THR:HG23	2.06	0.55
22:BA:2100:G:O6	22:BA:2189:U:O4	2.25	0.55
4:AD:50:ASP:HA	4:AD:53:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:104:ARG:HG2	4:AD:104:ARG:HH11	1.71	0.55
23:BB:1:U:H2'	23:BB:2:G:H8	1.71	0.55
1:AA:1012:A:N6	1:AA:1018:G:O6	2.39	0.55
49:B1:9:ILE:HG21	49:B1:51:GLU:OE1	2.07	0.55
55:B8:37:1MG:H2'	55:B8:38:A:C8	2.42	0.55
2:AB:204:ASP:C	2:AB:205:ASP:OD1	2.45	0.55
22:BA:2182:U:H2'	22:BA:2183:A:C8	2.42	0.55
4:AD:95:GLU:HA	4:AD:100:ASN:HD22	1.72	0.54
18:AR:26:ILE:HG22	18:AR:30:LYS:NZ	2.21	0.54
27:BF:135:GLN:HE21	27:BF:149:VAL:HA	1.71	0.54
1:AA:1008:U:H1'	1:AA:1009:U:C6	2.42	0.54
29:BH:104:THR:HA	29:BH:107:GLY:H	1.72	0.54
29:BH:114:GLU:OE1	29:BH:114:GLU:N	2.41	0.54
9:AI:47:VAL:HA	9:AI:50:GLN:HE21	1.71	0.54
22:BA:646:U:C5	22:BA:2368:C:H1'	2.42	0.54
48:B0:38:HIS:ND1	48:B0:39:LEU:O	2.39	0.54
1:AA:390:U:H2'	1:AA:391:G:H8	1.73	0.54
21:AU:31:GLU:O	21:AU:35:ARG:HG3	2.07	0.54
22:BA:1223:G:OP1	39:BR:68:ARG:NH1	2.39	0.54
3:AC:184:TYR:O	3:AC:185:ASN:ND2	2.41	0.54
5:AE:115:LEU:HD13	5:AE:123:VAL:HG21	1.90	0.54
22:BA:358:U:C2	22:BA:359:G:C8	2.96	0.54
22:BA:832:U:H2'	22:BA:833:A:H8	1.72	0.54
18:AR:26:ILE:CG2	18:AR:30:LYS:NZ	2.71	0.54
22:BA:2128:G:H2'	22:BA:2129:C:H6	1.72	0.54
22:BA:2796:U:H2'	22:BA:2797:U:H2'	1.89	0.54
1:AA:1088:G:H21	1:AA:1167:A:H61	1.54	0.54
1:AA:1320:C:C5'	19:AS:3:ARG:HH12	2.20	0.54
22:BA:414:C:H2'	22:BA:415:A:H8	1.73	0.54
35:BN:114:GLU:OE1	35:BN:118:ARG:NH1	2.41	0.54
1:AA:280:C:H42	17:AQ:39:LYS:NZ	2.05	0.54
1:AA:714:G:H2'	1:AA:715:A:C8	2.43	0.54
5:AE:111:MET:CE	5:AE:125:ALA:HB1	2.38	0.54
22:BA:2394:C:H5"	33:BL:63:LYS:HE2	1.90	0.54
17:AQ:39:LYS:O	17:AQ:39:LYS:HG3	2.08	0.54
22:BA:281:C:H2'	22:BA:282:A:C8	2.43	0.54
25:BD:156:PHE:CE1	31:BJ:81:ILE:HD13	2.42	0.54
41:BT:11:LEU:O	46:BY:29:ARG:NH1	2.41	0.54
55:B8:71:C:H2'	55:B8:72:G:C8	2.43	0.54
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.90	0.53
9:AI:46:MET:O	9:AI:50:GLN:HG2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2522:U:O2'	22:BA:2647:U:OP1	2.21	0.53
10:AJ:16:ARG:HG2	10:AJ:16:ARG:HH11	1.73	0.53
24:BC:133:ARG:NE	24:BC:187:ASP:OD1	2.39	0.53
1:AA:946:A:H2'	1:AA:947:G:C8	2.44	0.53
2:AB:223:GLU:HA	2:AB:226:SER:HB3	1.89	0.53
22:BA:1738:G:HO2'	22:BA:1739:A:H8	1.56	0.53
27:BF:38:MET:HE2	27:BF:152:LEU:HB3	1.91	0.53
1:AA:1533:C:N3	21:AU:54:LYS:NZ	2.55	0.53
2:AB:45:LYS:O	2:AB:49:MET:HG2	2.09	0.53
15:AO:76:ALA:O	15:AO:80:GLN:HG3	2.09	0.53
22:BA:685:A:OP2	60:BA:3411:HOH:O	2.19	0.53
55:B8:66:A:H2'	55:B8:67:U:C6	2.43	0.53
8:AH:88:ARG:HB2	8:AH:91:GLU:OE1	2.09	0.53
9:AI:87:LEU:HD11	9:AI:98:LEU:HD21	1.91	0.53
41:BT:67:VAL:HG22	41:BT:76:ARG:HG3	1.91	0.53
9:AI:80:ARG:HH21	9:AI:103:PHE:HA	1.74	0.53
11:AK:53:ARG:NH1	11:AK:53:ARG:HA	2.24	0.53
22:BA:2291:U:H2'	22:BA:2292:U:C6	2.43	0.53
3:AC:36:ASP:OD1	3:AC:59:ARG:NH2	2.41	0.53
4:AD:97:ARG:O	4:AD:101:VAL:HG23	2.09	0.53
22:BA:78:U:H2'	22:BA:79:C:C6	2.44	0.53
22:BA:1009:A:OP1	31:BJ:39:LYS:NZ	2.41	0.53
22:BA:2185:U:H2'	22:BA:2186:G:H8	1.73	0.53
1:AA:212:G:H2'	1:AA:213:G:C8	2.43	0.53
4:AD:82:LEU:HB2	4:AD:89:ASN:HD22	1.73	0.53
4:AD:101:VAL:O	4:AD:105:MET:HG3	2.09	0.53
11:AK:97:ILE:HG22	21:AU:12:PHE:HZ	1.73	0.53
22:BA:140:C:H5'	22:BA:141:G:C8	2.44	0.53
22:BA:2191:A:H2'	22:BA:2192:U:C6	2.44	0.53
22:BA:2246:G:H2'	22:BA:2247:A:C8	2.44	0.53
22:BA:2250:G:O2'	22:BA:2496:C:OP1	2.26	0.53
44:BW:40:GLN:HB2	44:BW:44:LYS:CE	2.38	0.53
1:AA:717:U:H4'	11:AK:119:ASN:HD22	1.73	0.52
18:AR:39:ILE:HD12	18:AR:59:ILE:HD12	1.91	0.52
22:BA:1348:C:OP1	60:BA:3410:HOH:O	2.19	0.52
29:BH:104:THR:HG21	29:BH:110:VAL:H	1.74	0.52
1:AA:87:C:H2'	1:AA:88:U:H4'	1.91	0.52
1:AA:171:A:H2'	1:AA:172:A:C8	2.44	0.52
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.91	0.52
1:AA:1530:G:N7	21:AU:46:LYS:NZ	2.57	0.52
2:AB:208:ARG:HA	2:AB:211:THR:OG1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:26:PHE:HD1	7:AG:101:MET:HG2	1.73	0.52
22:BA:2478:A:OP2	52:B4:2:LYS:NZ	2.26	0.52
2:AB:76:ALA:O	2:AB:80:VAL:HG23	2.09	0.52
3:AC:35:SER:O	3:AC:39:VAL:HG12	2.09	0.52
4:AD:65:TYR:CD2	4:AD:94:LEU:HB3	2.44	0.52
22:BA:1177:G:H2'	22:BA:1178:C:C6	2.44	0.52
22:BA:1543:G:HO2'	22:BA:1544:A:H8	1.55	0.52
26:BE:47:LYS:HA	26:BE:51:GLU:OE1	2.09	0.52
12:AL:94:ARG:HG3	12:AL:94:ARG:NH1	2.25	0.52
19:AS:5:LEU:HD12	19:AS:5:LEU:H	1.74	0.52
22:BA:585:G:N7	38:BQ:6:ARG:NH2	2.56	0.52
1:AA:384:G:H2'	1:AA:385:C:C6	2.44	0.52
1:AA:1279:G:OP1	10:AJ:9:ARG:NH2	2.42	0.52
2:AB:130:THR:O	2:AB:131:LYS:HB2	2.10	0.52
13:AM:107:ARG:NH2	13:AM:113:ARG:HA	2.25	0.52
1:AA:529:G:H5'	1:AA:530:G:OP2	2.09	0.52
9:AI:80:ARG:NH2	9:AI:103:PHE:HA	2.24	0.52
22:BA:456:C:O2'	41:BT:73:ARG:NH1	2.41	0.52
27:BF:94:GLU:O	27:BF:98:GLU:HG3	2.09	0.52
33:BL:69:ARG:HG2	33:BL:69:ARG:NH1	2.24	0.52
1:AA:745:G:H2'	1:AA:746:A:C8	2.44	0.52
9:AI:12:ARG:HG3	9:AI:77:GLY:HA3	1.92	0.52
11:AK:19:GLY:O	11:AK:82:LEU:HA	2.09	0.52
13:AM:4:ILE:HG22	13:AM:5:ALA:N	2.25	0.52
22:BA:880:G:H2'	22:BA:881:G:H8	1.73	0.52
3:AC:34:ASP:OD1	3:AC:38:LYS:NZ	2.40	0.52
43:BV:64:VAL:HG22	43:BV:69:GLU:HG2	1.91	0.52
37:BP:32:VAL:HG23	37:BP:39:ARG:HG3	1.90	0.52
4:AD:160:GLU:OE1	4:AD:160:GLU:N	2.39	0.52
7:AG:24:ALA:O	7:AG:28:ASN:OD1	2.27	0.52
13:AM:98:ARG:HB2	13:AM:100:GLN:HE22	1.74	0.52
22:BA:1800:C:H3'	24:BC:146:MET:HE1	1.92	0.52
22:BA:2812:G:H2'	22:BA:2813:A:C8	2.45	0.52
1:AA:49:U:H5	1:AA:365:U:O4	1.89	0.51
1:AA:206:C:H2'	1:AA:207:C:C6	2.45	0.51
10:AJ:66:GLU:HB3	14:AN:99:ALA:HB2	1.91	0.51
27:BF:142:ASP:HB3	27:BF:145:LYS:HE2	1.92	0.51
1:AA:728:A:H2'	1:AA:729:A:C8	2.45	0.51
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.38	0.51
3:AC:130:PHE:O	3:AC:134:MET:HG3	2.09	0.51
7:AG:70:ARG:HG2	7:AG:100:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AT:2:ALA:HB3	20:AT:8:LYS:HG3	1.93	0.51
22:BA:1662:U:OP2	60:BA:3413:HOH:O	2.19	0.51
34:BM:75:GLU:HG3	34:BM:90:GLU:HG3	1.92	0.51
19:AS:12:ASP:OD2	19:AS:35:SER:OG	2.08	0.51
22:BA:1485:U:H2'	22:BA:1486:U:C6	2.46	0.51
28:BG:8:PRO:HB3	28:BG:51:THR:HG22	1.91	0.51
29:BH:8:LYS:CD	29:BH:14:SER:HB3	2.40	0.51
22:BA:1590:A:H2'	22:BA:1591:A:C8	2.45	0.51
31:BJ:95:ARG:HD2	31:BJ:96:ARG:NH1	2.25	0.51
1:AA:713:G:H2'	1:AA:714:G:C8	2.45	0.51
1:AA:1318:A:H1'	19:AS:37:ARG:CZ	2.40	0.51
13:AM:4:ILE:HG23	13:AM:57:ARG:HG2	1.93	0.51
1:AA:126:G:OP1	1:AA:605:U:O2'	2.24	0.51
1:AA:450:G:H5'	1:AA:451:A:H5"	1.92	0.51
1:AA:539:A:H2'	1:AA:540:G:H8	1.75	0.51
16:AP:52:LEU:HD21	16:AP:75:ILE:HG12	1.93	0.51
22:BA:2316:G:H2'	22:BA:2317:A:H8	1.76	0.51
27:BF:94:GLU:OE2	27:BF:98:GLU:CD	2.49	0.51
45:BX:69:ALA:HA	45:BX:72:ARG:HE	1.76	0.51
7:AG:75:VAL:CG1	7:AG:86:GLN:HB3	2.41	0.51
1:AA:269:C:H2'	1:AA:270:A:C8	2.44	0.51
1:AA:390:U:H2'	1:AA:391:G:C8	2.46	0.51
1:AA:524:G:H2'	1:AA:525:C:C6	2.45	0.51
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.46	0.51
2:AB:6:MET:CE	2:AB:43:LEU:HB3	2.40	0.51
9:AI:60:LYS:HE3	9:AI:61:LEU:HD23	1.93	0.51
18:AR:61:ARG:HG3	18:AR:61:ARG:HH11	1.76	0.51
22:BA:2447:G:H1'	60:BA:4636:HOH:O	2.11	0.51
55:B8:62:C:H2'	55:B8:63:U:C6	2.46	0.51
6:AF:103:VAL:O	6:AF:106:LYS:HB2	2.11	0.51
22:BA:1796:U:H2'	22:BA:1797:G:H8	1.75	0.51
22:BA:2046:G:OP2	60:BA:3412:HOH:O	2.19	0.51
32:BK:38:ILE:HD11	32:BK:112:PHE:HZ	1.74	0.51
55:B8:69:A:H2'	55:B8:70:C:C6	2.46	0.51
1:AA:579:A:O2'	15:AO:54:ARG:NH1	2.43	0.51
1:AA:600:A:H5"	8:AH:89:LYS:HD3	1.93	0.51
1:AA:1033:G:H2'	1:AA:1034:G:C8	2.46	0.51
2:AB:187:VAL:HG11	2:AB:199:VAL:HG13	1.93	0.51
12:AL:4:VAL:HG13	17:AQ:34:TYR:HB3	1.93	0.51
22:BA:1079:C:H2'	22:BA:1080:A:H8	1.76	0.51
24:BC:78:VAL:HG21	24:BC:110:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BT:6:ARG:HD2	41:BT:6:ARG:O	2.10	0.51
2:AB:8:ASP:OD1	2:AB:9:MET:N	2.43	0.50
5:AE:82:GLN:HB2	5:AE:83:HIS:HD2	1.76	0.50
8:AH:106:THR:CG2	8:AH:121:LEU:HB3	2.40	0.50
22:BA:1100:C:H2'	22:BA:1101:U:O4'	2.11	0.50
22:BA:1570:A:H2'	22:BA:1571:A:C8	2.46	0.50
30:BI:14:ALA:HB1	30:BI:34:LEU:CD2	2.40	0.50
53:B5:14:ASN:O	53:B5:20:VAL:HG21	2.11	0.50
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.76	0.50
22:BA:1300:G:H4'	22:BA:1301:A:H5"	1.93	0.50
1:AA:1317:C:C4	14:AN:53:ARG:HD2	2.46	0.50
2:AB:18:HIS:CE1	2:AB:205:ASP:OD2	2.64	0.50
2:AB:60:ILE:HA	2:AB:63:ARG:HH21	1.76	0.50
8:AH:106:THR:HG22	8:AH:107:SER:H	1.76	0.50
8:AH:106:THR:HG23	8:AH:122:GLY:O	2.12	0.50
22:BA:959:A:H2'	22:BA:960:A:C8	2.46	0.50
28:BG:24:ILE:HD11	28:BG:43:VAL:CG1	2.36	0.50
4:AD:56:ARG:HA	4:AD:56:ARG:NE	2.23	0.50
7:AG:80:VAL:N	7:AG:83:SER:O	2.44	0.50
13:AM:54:ASP:HA	13:AM:57:ARG:HB2	1.93	0.50
1:AA:235:C:H2'	1:AA:236:A:C8	2.46	0.50
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.25	0.50
22:BA:608:A:H2'	22:BA:609:A:C8	2.47	0.50
1:AA:219:U:H2'	1:AA:220:G:H8	1.77	0.50
1:AA:890:G:O2'	1:AA:906:A:N6	2.44	0.50
22:BA:798:G:OP1	60:BA:3414:HOH:O	2.20	0.50
46:BY:19:LEU:O	46:BY:23:ARG:HD3	2.11	0.50
1:AA:80:A:H2'	1:AA:81:A:O4'	2.12	0.50
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.47	0.50
21:AU:39:GLU:OE2	21:AU:44:GLU:HG3	2.11	0.50
26:BE:7:ASP:OD2	26:BE:122:GLU:HB2	2.11	0.50
22:BA:848:C:H2'	22:BA:849:A:C8	2.47	0.50
22:BA:1870:C:O2'	22:BA:1871:A:O5'	2.30	0.50
25:BD:152:PRO:HG3	25:BD:156:PHE:CZ	2.47	0.50
6:AF:45:ARG:HD3	6:AF:59:TYR:CG	2.47	0.49
22:BA:191:A:H2'	22:BA:192:C:C6	2.47	0.49
30:BI:13:THR:HB	30:BI:23:LYS:HD3	1.92	0.49
32:BK:121:GLU:OE1	37:BP:65:SER:OG	2.29	0.49
1:AA:1314:C:H2'	1:AA:1315:U:H6	1.77	0.49
14:AN:46:LEU:HD11	19:AS:13:LEU:HB2	1.93	0.49
22:BA:172:A:H2'	22:BA:173:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:217:VAL:O	2:AB:221:VAL:HG13	2.11	0.49
7:AG:111:ARG:HH12	7:AG:123:GLU:N	2.10	0.49
19:AS:19:VAL:HG21	19:AS:44:MET:HB3	1.93	0.49
22:BA:276:U:H2'	22:BA:277:G:O4'	2.13	0.49
22:BA:879:G:H2'	22:BA:880:G:H8	1.76	0.49
22:BA:2193:G:H2'	22:BA:2194:U:C6	2.46	0.49
1:AA:674:G:H21	11:AK:118:HIS:HB2	1.78	0.49
22:BA:1173:U:O2'	22:BA:1174:U:O5'	2.30	0.49
1:AA:1130:A:H2'	1:AA:1131:G:C8	2.47	0.49
4:AD:124:MET:HG2	4:AD:146:ARG:HG3	1.95	0.49
9:AI:6:TYR:HB2	9:AI:21:ILE:CG1	2.43	0.49
19:AS:47:LEU:HD12	19:AS:48:THR:H	1.77	0.49
23:BB:51:G:OP1	36:BO:63:LYS:NZ	2.34	0.49
28:BG:102:VAL:HG22	28:BG:116:GLN:HG2	1.94	0.49
33:BL:57:LEU:HD22	51:B3:54:ASP:HB3	1.94	0.49
1:AA:426:U:P	4:AD:33:LYS:NZ	2.86	0.49
5:AE:13:GLU:OE2	5:AE:68:ARG:NH2	2.42	0.49
6:AF:70:VAL:HG23	6:AF:71:ILE:HD13	1.93	0.49
18:AR:61:ARG:HG3	18:AR:61:ARG:NH1	2.27	0.49
22:BA:833:A:H2'	22:BA:834:G:C8	2.47	0.49
22:BA:1386:C:H2'	22:BA:1387:A:C8	2.48	0.49
24:BC:180:GLU:OE2	24:BC:270:ARG:NH2	2.45	0.49
26:BE:23:PHE:CD1	26:BE:111:GLU:HG3	2.47	0.49
28:BG:117:LEU:HD11	28:BG:144:VAL:HG11	1.95	0.49
29:BH:16:GLY:HA2	29:BH:47:PHE:CE2	2.48	0.49
30:BI:30:HIS:CG	30:BI:31:ASP:N	2.80	0.49
4:AD:118:VAL:HG12	4:AD:123:ILE:HG13	1.94	0.49
22:BA:1590:A:H2'	22:BA:1591:A:H8	1.76	0.49
22:BA:2128:G:H2'	22:BA:2129:C:C6	2.47	0.49
1:AA:1112:C:O2'	3:AC:179:ARG:HD2	2.12	0.49
1:AA:1143:G:H2'	1:AA:1144:G:H8	1.78	0.49
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.61	0.49
13:AM:71:ARG:HG3	13:AM:71:ARG:HH11	1.77	0.49
22:BA:2334:U:H1'	36:BO:13:ARG:HD3	1.94	0.49
27:BF:63:GLN:HE21	27:BF:89:VAL:CG2	2.26	0.49
31:BJ:125:TYR:OH	31:BJ:132:HIS:NE2	2.38	0.49
1:AA:280:C:H42	17:AQ:39:LYS:HZ1	1.60	0.49
1:AA:891:U:H2'	1:AA:892:A:H8	1.76	0.49
1:AA:1414:U:H2'	1:AA:1415:G:H8	1.78	0.49
22:BA:545:U:O2'	22:BA:546:U:O4'	2.30	0.49
22:BA:1175:A:H8	22:BA:1176:U:C4	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2845:U:H5”	37:BP:52:ASN:O	2.13	0.49
42:BU:99:ASN:ND2	42:BU:101:GLU:OE2	2.45	0.49
55:B8:19:G:H4’	55:B8:20:U:OP2	2.11	0.49
1:AA:189:A:H2’	1:AA:190:A:C8	2.48	0.49
1:AA:880:C:OP1	12:AL:5:ASN:ND2	2.46	0.49
22:BA:2086:U:H2’	22:BA:2087:G:C8	2.48	0.49
22:BA:2305:U:H5”	27:BF:131:GLY:HA3	1.95	0.49
24:BC:145:GLU:HB2	24:BC:188:CYS:HB3	1.94	0.49
47:BZ:57:VAL:HG12	47:BZ:59:GLU:HG3	1.95	0.49
9:AI:22:LYS:HB2	9:AI:62:ASP:OD1	2.13	0.48
22:BA:1322:A:H5’	40:BS:11:ARG:NH2	2.28	0.48
34:BM:50:ARG:HD3	34:BM:65:ILE:HD11	1.94	0.48
43:BV:2:PHE:HB2	43:BV:61:LEU:HD22	1.95	0.48
1:AA:300:A:O5’	1:AA:300:A:H8	1.95	0.48
22:BA:1682:G:H2’	22:BA:1683:U:C6	2.47	0.48
22:BA:2313:C:H5”	27:BF:88:LYS:HD2	1.95	0.48
22:BA:2680:U:O2’	22:BA:2681:C:H5’	2.13	0.48
22:BA:2795:C:H2’	22:BA:2796:U:C6	2.48	0.48
11:AK:53:ARG:HH12	11:AK:57:LYS:CD	2.21	0.48
22:BA:594:U:H2’	22:BA:595:C:C6	2.49	0.48
22:BA:1485:U:H2’	22:BA:1486:U:H6	1.77	0.48
22:BA:2101:A:H2’	22:BA:2102:G:H8	1.78	0.48
1:AA:1412:C:H2’	1:AA:1413:A:C8	2.49	0.48
2:AB:115:LYS:O	2:AB:119:THR:HG22	2.14	0.48
4:AD:188:ARG:NH1	4:AD:192:SER:O	2.44	0.48
7:AG:50:LEU:CD2	7:AG:124:LEU:HB3	2.39	0.48
9:AI:28:ILE:HG21	9:AI:35:LEU:HD12	1.94	0.48
22:BA:194:G:H2’	22:BA:195:A:O4’	2.13	0.48
24:BC:155:ALA:HB2	24:BC:162:VAL:HG23	1.95	0.48
22:BA:703:U:H2’	22:BA:704:G:O4’	2.13	0.48
22:BA:1494:A:H2’	22:BA:1495:A:C8	2.49	0.48
1:AA:1088:G:N2	1:AA:1167:A:H61	2.10	0.48
3:AC:184:TYR:OH	3:AC:199:LYS:HD3	2.13	0.48
4:AD:99:ASP:OD1	4:AD:100:ASN:N	2.45	0.48
22:BA:358:U:H2’	22:BA:359:G:H8	1.77	0.48
22:BA:2334:U:O2’	36:BO:13:ARG:NH1	2.46	0.48
1:AA:674:G:H2’	1:AA:675:A:C8	2.48	0.48
5:AE:105:ILE:HB	5:AE:112:ARG:NH1	2.29	0.48
8:AH:96:MET:CG	8:AH:99:LEU:HB2	2.43	0.48
16:AP:6:LEU:HB3	16:AP:17:TYR:HD2	1.78	0.48
22:BA:2291:U:OP1	22:BA:2380:C:O2’	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2649:C:H2'	22:BA:2650:U:H6	1.79	0.48
34:BM:66:ARG:NH1	34:BM:104:GLU:OE2	2.46	0.48
10:AJ:80:THR:HG22	10:AJ:83:THR:HG23	1.95	0.48
22:BA:5:A:H2'	22:BA:6:A:C8	2.48	0.48
22:BA:419:U:OP1	60:BA:3416:HOH:O	2.20	0.48
22:BA:1809:A:H2'	22:BA:1810:A:C8	2.48	0.48
35:BN:35:LYS:HE2	35:BN:100:CYS:SG	2.53	0.48
1:AA:1297:G:O2'	7:AG:114:LYS:NZ	2.47	0.48
22:BA:1173:U:O2'	22:BA:1174:U:O4'	2.32	0.48
22:BA:1495:A:H2'	22:BA:1496:A:C8	2.49	0.48
22:BA:2728:U:HO2'	22:BA:2729:G:H8	1.60	0.48
24:BC:38:SER:OG	60:BC:401:HOH:O	2.14	0.48
1:AA:280:C:N4	17:AQ:39:LYS:NZ	2.62	0.48
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.49	0.48
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.49	0.48
1:AA:1464:U:H2'	1:AA:1465:A:H8	1.79	0.48
4:AD:95:GLU:HA	4:AD:100:ASN:ND2	2.29	0.48
9:AI:17:ALA:HB2	9:AI:67:VAL:HG12	1.95	0.48
9:AI:63:LEU:HD12	9:AI:65:ILE:HD11	1.96	0.48
15:AO:70:LEU:HD11	15:AO:77:ARG:HB3	1.95	0.48
22:BA:2193:G:H2'	22:BA:2194:U:H6	1.78	0.48
32:BK:111:LYS:HG2	32:BK:112:PHE:CE1	2.49	0.48
1:AA:131:A:H2'	1:AA:132:C:C6	2.49	0.47
1:AA:868:C:H2'	1:AA:869:G:O4'	2.13	0.47
1:AA:1273:C:H2'	1:AA:1274:A:O4'	2.14	0.47
22:BA:645:C:H2'	22:BA:647:G:C8	2.49	0.47
22:BA:1102:C:H2'	22:BA:1103:A:H8	1.78	0.47
2:AB:165:ASP:OD2	2:AB:168:HIS:HB2	2.14	0.47
6:AF:23:GLU:HA	6:AF:26:THR:OG1	2.14	0.47
22:BA:347:A:H2'	22:BA:348:A:C8	2.49	0.47
22:BA:1729:U:O2	22:BA:1731:G:N2	2.38	0.47
1:AA:674:G:H2'	1:AA:675:A:H8	1.80	0.47
9:AI:5:GLN:HE22	9:AI:22:LYS:HD2	1.79	0.47
34:BM:50:ARG:O	34:BM:54:THR:HG22	2.14	0.47
55:B8:23:C:H2'	55:B8:24:G:H8	1.79	0.47
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.43	0.47
3:AC:127:ARG:HH11	3:AC:127:ARG:CB	2.26	0.47
22:BA:589:U:H2'	22:BA:590:A:C8	2.49	0.47
1:AA:337:G:H2'	1:AA:338:A:H8	1.80	0.47
22:BA:1322:A:H5'	40:BS:11:ARG:HH21	1.80	0.47
22:BA:2071:A:H2'	22:BA:2072:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2311:A:N3	27:BF:85:ILE:HD11	2.30	0.47
22:BA:2788:C:H2'	22:BA:2789:C:C6	2.50	0.47
29:BH:68:ARG:HH21	29:BH:134:VAL:HB	1.79	0.47
34:BM:41:LEU:HG	34:BM:96:ILE:HG13	1.95	0.47
22:BA:1047:G:O2'	22:BA:1110:G:N1	2.41	0.47
22:BA:1799:G:OP1	24:BC:258:ARG:NH1	2.40	0.47
22:BA:2100:G:C2	22:BA:2101:A:H1'	2.49	0.47
29:BH:122:LEU:HD12	29:BH:122:LEU:O	2.15	0.47
1:AA:1218:C:H2'	1:AA:1219:A:H8	1.79	0.47
1:AA:1315:U:O2	1:AA:1360:A:H2	1.97	0.47
2:AB:53:ALA:O	2:AB:57:LEU:HD12	2.14	0.47
3:AC:110:GLU:HB2	3:AC:144:LEU:HD12	1.97	0.47
9:AI:7:TYR:CE1	9:AI:18:ARG:HB2	2.49	0.47
19:AS:29:LYS:H	19:AS:29:LYS:HD2	1.79	0.47
22:BA:1059:G:H2'	22:BA:1060:U:C5	2.49	0.47
22:BA:1720:U:H2'	22:BA:1721:G:O4'	2.14	0.47
22:BA:2455:G:H2'	22:BA:2456:C:C6	2.49	0.47
27:BF:38:MET:CE	27:BF:151:GLY:O	2.62	0.47
35:BN:35:LYS:HG3	35:BN:112:TYR:CE1	2.50	0.47
50:B2:12:ARG:NH2	50:B2:44:VAL:HG21	2.30	0.47
1:AA:696:A:H2'	1:AA:697:U:H6	1.80	0.47
1:AA:1279:G:P	10:AJ:9:ARG:HH22	2.38	0.47
2:AB:212:LEU:HD12	2:AB:213:TYR:N	2.30	0.47
4:AD:101:VAL:HG21	4:AD:137:VAL:HG21	1.96	0.47
13:AM:71:ARG:HG3	13:AM:71:ARG:NH1	2.29	0.47
15:AO:20:ASN:OD1	15:AO:21:ASP:N	2.48	0.47
22:BA:588:U:H2'	22:BA:589:U:C6	2.50	0.47
29:BH:50:ARG:HG3	29:BH:53:GLU:OE2	2.15	0.47
55:B8:23:C:H2'	55:B8:24:G:C8	2.50	0.47
6:AF:72:ASP:OD1	6:AF:73:GLU:N	2.47	0.47
7:AG:50:LEU:CD1	7:AG:121:ALA:HA	2.43	0.47
22:BA:646:U:H5	22:BA:2368:C:H1'	1.80	0.47
44:BW:40:GLN:HB2	44:BW:44:LYS:CD	2.44	0.47
1:AA:1225:A:OP1	13:AM:102:THR:HG22	2.15	0.47
22:BA:1334:G:OP1	41:BT:69:ARG:NH2	2.48	0.47
22:BA:2514:U:H2'	22:BA:2515:C:C6	2.50	0.47
25:BD:61:THR:HB	25:BD:63:PRO:HD2	1.97	0.47
3:AC:155:GLY:O	3:AC:196:ILE:HG12	2.14	0.46
16:AP:52:LEU:CD2	16:AP:75:ILE:HG12	2.46	0.46
22:BA:2278:A:OP1	34:BM:10:ARG:NH2	2.46	0.46
32:BK:63:VAL:HG12	32:BK:107:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:695:A:H2'	1:AA:696:A:C8	2.51	0.46
2:AB:18:HIS:H	2:AB:189:THR:HG22	1.79	0.46
20:AT:81:ALA:O	20:AT:85:LYS:HD3	2.15	0.46
22:BA:64:A:H2'	22:BA:65:U:C6	2.51	0.46
22:BA:1796:U:H2'	22:BA:1797:G:C8	2.49	0.46
32:BK:105:ARG:HG2	32:BK:108:ARG:CD	2.44	0.46
55:B8:51:A:H2'	55:B8:52:G:C8	2.50	0.46
3:AC:159:GLY:HA2	3:AC:193:TYR:CD2	2.50	0.46
22:BA:141:G:N2	22:BA:142:A:C8	2.83	0.46
22:BA:1370:C:H2'	22:BA:1371:G:O4'	2.15	0.46
22:BA:2567:G:H2'	22:BA:2568:U:C6	2.50	0.46
22:BA:2649:C:H2'	22:BA:2650:U:C6	2.51	0.46
24:BC:148:PRO:HG2	24:BC:185:GLU:OE2	2.15	0.46
28:BG:24:ILE:CD1	28:BG:43:VAL:HG11	2.36	0.46
29:BH:81:ALA:HB1	29:BH:149:GLU:CG	2.39	0.46
1:AA:1175:G:H2'	1:AA:1176:A:H8	1.80	0.46
1:AA:1176:A:H2'	1:AA:1177:G:C8	2.50	0.46
7:AG:60:GLU:O	7:AG:64:VAL:HG22	2.15	0.46
13:AM:49:SER:HB3	13:AM:52:GLN:HG3	1.98	0.46
22:BA:280:U:H2'	22:BA:281:C:C6	2.50	0.46
22:BA:2100:G:C6	22:BA:2101:A:C4	3.03	0.46
25:BD:105:LYS:HA	25:BD:105:LYS:HD3	1.60	0.46
1:AA:1239:A:H62	1:AA:1299:A:H62	1.64	0.46
1:AA:1363:A:O2'	1:AA:1365:G:N7	2.40	0.46
5:AE:86:LYS:HD3	5:AE:95:PHE:HB2	1.97	0.46
10:AJ:40:ILE:O	10:AJ:72:ARG:HD3	2.15	0.46
10:AJ:40:ILE:CG2	10:AJ:73:LEU:HB3	2.43	0.46
22:BA:593:U:H2'	22:BA:594:U:C6	2.50	0.46
22:BA:2255:G:O2'	55:B8:3:G:OP2	2.25	0.46
7:AG:74:GLU:O	7:AG:88:PRO:HA	2.15	0.46
22:BA:363:G:H2'	22:BA:364:C:C6	2.50	0.46
22:BA:2585:U:C2	53:B5:24:PRO:HG3	2.51	0.46
1:AA:751:U:H2'	1:AA:752:G:O4'	2.16	0.46
3:AC:121:THR:HB	3:AC:189:ALA:HB2	1.97	0.46
12:AL:87:VAL:HG11	12:AL:90:LEU:HD12	1.98	0.46
22:BA:2130:U:O2'	22:BA:2133:G:O2'	2.29	0.46
22:BA:2591:C:H2'	22:BA:2592:G:C8	2.50	0.46
22:BA:2740:A:H2'	22:BA:2741:A:C8	2.51	0.46
31:BJ:49:ASP:OD1	31:BJ:121:LYS:NZ	2.47	0.46
43:BV:6:ALA:HB2	43:BV:42:LEU:HD23	1.97	0.46
1:AA:89:U:H2'	1:AA:90:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:122:G:OP2	1:AA:122:G:H8	1.98	0.46
2:AB:108:ARG:HA	2:AB:111:ILE:HG12	1.97	0.46
3:AC:39:VAL:O	3:AC:43:LEU:HD13	2.15	0.46
14:AN:15:LEU:HD22	14:AN:54:ASP:HB2	1.97	0.46
15:AO:74:ASP:OD2	15:AO:77:ARG:NH1	2.48	0.46
22:BA:357:C:H2'	22:BA:358:U:C6	2.50	0.46
22:BA:2099:U:H2'	22:BA:2100:G:O5'	2.16	0.46
29:BH:135:HIS:HB3	29:BH:138:VAL:HB	1.97	0.46
1:AA:883:C:O2'	1:AA:884:U:H5'	2.16	0.46
4:AD:169:THR:HG23	4:AD:184:ARG:HH22	1.81	0.46
22:BA:828:U:H2'	22:BA:829:A:C8	2.51	0.46
22:BA:1802:A:H2'	22:BA:1803:A:C8	2.51	0.46
27:BF:10:ASP:OD1	27:BF:11:GLU:N	2.49	0.46
31:BJ:7:LYS:O	31:BJ:11:VAL:HG13	2.15	0.46
32:BK:40:LYS:HD3	32:BK:58:LEU:O	2.16	0.46
34:BM:135:VAL:HG13	43:BV:57:TYR:CD2	2.51	0.46
1:AA:478:A:OP2	1:AA:479:U:H5"	2.16	0.46
5:AE:134:ILE:O	5:AE:138:ARG:HG2	2.16	0.46
21:AU:25:LYS:HE3	21:AU:25:LYS:HB3	1.68	0.46
1:AA:719:C:O2	18:AR:39:ILE:HG22	2.16	0.45
1:AA:753:A:OP1	15:AO:69:TYR:OH	2.34	0.45
4:AD:19:LEU:HD22	4:AD:64:ILE:HG13	1.97	0.45
7:AG:75:VAL:HG11	7:AG:86:GLN:HB3	1.98	0.45
22:BA:1484:U:H2'	22:BA:1485:U:C6	2.51	0.45
39:BR:60:LYS:N	39:BR:60:LYS:HD3	2.30	0.45
1:AA:908:A:H2'	1:AA:909:A:C8	2.51	0.45
22:BA:396:G:OP2	45:BX:10:LYS:NZ	2.46	0.45
22:BA:2251:OMG:HM23	22:BA:2251:OMG:H1'	1.64	0.45
41:BT:53:VAL:CG1	41:BT:54:GLU:N	2.79	0.45
49:B1:6:ARG:HG3	49:B1:24:THR:HB	1.98	0.45
1:AA:501:C:H2'	1:AA:502:A:C8	2.51	0.45
1:AA:954:G:H21	1:AA:1227:A:H62	1.63	0.45
1:AA:1122:U:H2'	1:AA:1123:U:C6	2.51	0.45
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.51	0.45
23:BB:48:U:H2'	23:BB:49:C:C6	2.51	0.45
44:BW:65:GLY:HA2	44:BW:85:GLU:HG3	1.99	0.45
1:AA:918:A:H2'	1:AA:919:A:C8	2.52	0.45
4:AD:114:ALA:O	4:AD:118:VAL:HG13	2.15	0.45
1:AA:413:G:H1'	1:AA:428:G:N2	2.31	0.45
1:AA:426:U:OP1	4:AD:33:LYS:NZ	2.49	0.45
1:AA:672:U:H2'	1:AA:673:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:45:ARG:HD3	6:AF:59:TYR:HB2	1.98	0.45
15:AO:71:LYS:HE3	15:AO:71:LYS:HB3	1.77	0.45
44:BW:41:ARG:NH2	60:BW:101:HOH:O	2.42	0.45
46:BY:19:LEU:HD12	46:BY:19:LEU:HA	1.77	0.45
55:B8:25:C:H2'	55:B8:26:A:O4'	2.17	0.45
1:AA:426:U:H2'	1:AA:427:U:C6	2.52	0.45
1:AA:1040:U:H2'	1:AA:1041:G:C8	2.49	0.45
4:AD:166:GLU:N	4:AD:166:GLU:OE1	2.49	0.45
8:AH:22:LYS:HB2	8:AH:22:LYS:HE2	1.63	0.45
10:AJ:59:LYS:NZ	10:AJ:62:ARG:HH22	2.14	0.45
22:BA:730:A:H5'	60:BA:3766:HOH:O	2.16	0.45
22:BA:1357:C:H2'	22:BA:1358:G:O4'	2.16	0.45
22:BA:1808:A:H3'	22:BA:1809:A:C8	2.52	0.45
22:BA:1923:U:H2'	22:BA:1924:C:C6	2.52	0.45
22:BA:2223:G:O3'	24:BC:265:LYS:HE3	2.16	0.45
25:BD:108:ASP:OD1	25:BD:173:GLN:HA	2.16	0.45
37:BP:6:LYS:HD3	37:BP:6:LYS:HA	1.66	0.45
55:B8:63:U:H2'	55:B8:64:C:C6	2.52	0.45
1:AA:1120:C:H2'	1:AA:1121:U:H6	1.81	0.45
4:AD:118:VAL:O	4:AD:131:ASN:HA	2.17	0.45
22:BA:369:U:O2'	60:BA:3415:HOH:O	2.20	0.45
22:BA:927:A:H2'	22:BA:928:A:C8	2.51	0.45
22:BA:2100:G:O6	22:BA:2189:U:C4	2.70	0.45
2:AB:5:SER:O	2:AB:9:MET:HG3	2.17	0.45
2:AB:45:LYS:O	2:AB:48:PRO:HD2	2.17	0.45
7:AG:130:ASN:O	7:AG:130:ASN:ND2	2.48	0.45
19:AS:11:ILE:HG13	19:AS:38:SER:HB2	1.98	0.45
22:BA:359:G:C5	22:BA:360:U:C5	3.05	0.45
30:BI:14:ALA:HA	30:BI:32:LEU:O	2.17	0.45
44:BW:41:ARG:NE	60:BW:101:HOH:O	2.41	0.45
7:AG:49:THR:O	7:AG:53:ARG:HB2	2.16	0.45
22:BA:438:G:H2'	22:BA:439:A:C8	2.52	0.45
40:BS:73:LYS:HB2	40:BS:106:VAL:HB	1.98	0.45
1:AA:719:C:H2'	18:AR:39:ILE:HG23	1.98	0.45
8:AH:112:THR:HG22	8:AH:114:ARG:H	1.82	0.45
22:BA:1746:A:H2'	22:BA:1747:U:C6	2.52	0.45
22:BA:2662:A:O5'	22:BA:2662:A:H8	2.00	0.45
31:BJ:31:GLU:OE1	31:BJ:34:ARG:HD3	2.17	0.45
1:AA:715:A:H2'	1:AA:716:A:C8	2.53	0.44
1:AA:1358:U:OP1	14:AN:75:ARG:HB2	2.16	0.44
22:BA:191:A:H2'	22:BA:192:C:H6	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1428:C:C5	22:BA:1569:A:H5"	2.52	0.44
22:BA:1794:A:H2'	22:BA:1795:C:C6	2.52	0.44
35:BN:57:THR:HG23	35:BN:62:ASN:ND2	2.32	0.44
41:BT:7:LEU:HD22	41:BT:46:ALA:HB2	1.99	0.44
1:AA:900:A:H2'	1:AA:901:A:C8	2.52	0.44
5:AE:105:ILE:HB	5:AE:112:ARG:HH12	1.82	0.44
8:AH:106:THR:CG2	8:AH:107:SER:N	2.80	0.44
21:AU:13:ASP:OD2	21:AU:17:ARG:NH2	2.51	0.44
22:BA:581:C:H2'	22:BA:582:A:C8	2.52	0.44
22:BA:1102:C:C2	22:BA:1103:A:C8	3.05	0.44
22:BA:1432:G:H2'	22:BA:1433:A:C8	2.52	0.44
22:BA:1819:A:H3'	24:BC:177:ARG:HG2	1.99	0.44
29:BH:41:LYS:HG3	29:BH:41:LYS:O	2.17	0.44
2:AB:23:TRP:CZ3	2:AB:25:PRO:HA	2.51	0.44
2:AB:32:PHE:HD2	2:AB:42:ASN:ND2	2.16	0.44
16:AP:76:LYS:O	16:AP:80:LYS:HD3	2.18	0.44
22:BA:363:G:H2'	22:BA:364:C:H6	1.83	0.44
22:BA:813:U:H2'	22:BA:814:C:C6	2.52	0.44
22:BA:1069:A:H4'	22:BA:1070:A:H5"	2.00	0.44
43:BV:55:GLU:O	43:BV:59:GLU:HG2	2.17	0.44
1:AA:31:G:O2'	1:AA:48:C:N4	2.49	0.44
1:AA:662:U:H2'	1:AA:663:A:C8	2.51	0.44
1:AA:1404:C:H2'	1:AA:1405:G:C8	2.52	0.44
6:AF:102:MET:HE1	18:AR:24:LYS:HB3	2.00	0.44
13:AM:29:ARG:O	13:AM:33:ILE:HG12	2.17	0.44
15:AO:73:LYS:HA	15:AO:73:LYS:HD2	1.80	0.44
19:AS:32:ARG:HG2	19:AS:57:HIS:CE1	2.51	0.44
22:BA:1548:A:H2'	22:BA:1549:A:C8	2.52	0.44
24:BC:120:VAL:HG22	29:BH:91:PHE:HB3	1.99	0.44
1:AA:320:A:H2'	1:AA:321:A:O4'	2.18	0.44
1:AA:363:A:OP2	12:AL:31:ARG:NE	2.50	0.44
1:AA:1342:C:H4'	9:AI:127:PHE:O	2.17	0.44
13:AM:19:LEU:CD1	13:AM:34:LEU:HD11	2.48	0.44
14:AN:83:LYS:HD2	14:AN:83:LYS:HA	1.66	0.44
36:BO:40:ILE:HD13	36:BO:47:VAL:HG22	2.00	0.44
1:AA:1456:A:H2'	1:AA:1457:G:O4'	2.17	0.44
2:AB:118:GLU:O	2:AB:121:SER:OG	2.24	0.44
8:AH:50:LYS:HE3	8:AH:60:GLU:HB3	2.00	0.44
9:AI:22:LYS:HE2	9:AI:62:ASP:OD1	2.18	0.44
10:AJ:6:ILE:HD12	10:AJ:102:LEU:HA	1.99	0.44
13:AM:49:SER:O	13:AM:53:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:720:U:H2'	22:BA:721:A:C8	2.53	0.44
22:BA:1028:A:N6	22:BA:1125:G:H2'	2.32	0.44
22:BA:1292:G:H2'	22:BA:1293:C:C6	2.52	0.44
32:BK:70:ARG:HD3	32:BK:76:VAL:HG22	1.99	0.44
34:BM:74:THR:O	34:BM:75:GLU:HG2	2.18	0.44
40:BS:70:LYS:HB2	40:BS:70:LYS:NZ	2.33	0.44
1:AA:1140:C:HO2'	1:AA:1141:C:H6	1.65	0.44
2:AB:145:GLU:HG2	2:AB:149:GLY:HA3	1.98	0.44
3:AC:131:ARG:NH2	3:AC:166:GLU:OE2	2.50	0.44
9:AI:6:TYR:HB2	9:AI:21:ILE:HG13	1.99	0.44
22:BA:2074:U:H2'	22:BA:2075:U:C6	2.52	0.44
29:BH:75:LEU:HD23	29:BH:106:ALA:HB1	1.98	0.44
1:AA:335:C:H2'	1:AA:336:A:C8	2.53	0.44
1:AA:384:G:H2'	1:AA:385:C:H6	1.82	0.44
2:AB:177:ASN:HD21	2:AB:195:GLY:CA	2.30	0.44
2:AB:210:VAL:O	2:AB:214:LEU:HD12	2.18	0.44
22:BA:1141:U:H4'	22:BA:1142:A:O4'	2.17	0.44
32:BK:105:ARG:HG2	32:BK:108:ARG:NE	2.33	0.44
1:AA:91:U:H2'	1:AA:92:U:O4'	2.17	0.44
1:AA:456:A:H2'	1:AA:457:G:C8	2.53	0.44
11:AK:84:VAL:HG11	11:AK:97:ILE:CD1	2.48	0.44
20:AT:43:ASP:OD2	20:AT:46:ALA:HB3	2.17	0.44
22:BA:358:U:H2'	22:BA:359:G:C8	2.53	0.44
26:BE:22:ASP:OD1	26:BE:23:PHE:N	2.51	0.44
2:AB:82:ASP:O	2:AB:86:SER:HB3	2.18	0.43
3:AC:79:LYS:O	3:AC:80:LYS:HB3	2.18	0.43
5:AE:39:VAL:HG13	5:AE:71:MET:CE	2.48	0.43
10:AJ:84:VAL:HG13	10:AJ:85:ASP:N	2.32	0.43
16:AP:23:ASP:HB3	16:AP:26:ASN:OD1	2.17	0.43
20:AT:28:MET:HE1	20:AT:66:LEU:HD22	1.98	0.43
20:AT:69:LYS:HB2	20:AT:69:LYS:HE2	1.73	0.43
22:BA:1703:G:H2'	22:BA:1704:C:C6	2.52	0.43
22:BA:2557:G:H2'	22:BA:2558:C:C6	2.53	0.43
22:BA:2801:G:H2'	22:BA:2802:G:H8	1.82	0.43
25:BD:7:LYS:HD3	25:BD:198:GLY:HA2	1.99	0.43
39:BR:58:VAL:HG12	39:BR:60:LYS:HD3	2.00	0.43
1:AA:78:A:C6	1:AA:79:G:C6	3.06	0.43
1:AA:85:U:H4'	1:AA:86:G:H4'	1.99	0.43
1:AA:335:C:H2'	1:AA:336:A:H8	1.83	0.43
1:AA:684:U:C1'	11:AK:40:ASN:HD22	2.31	0.43
1:AA:981:U:O2'	14:AN:61:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:102:THR:HG23	2:AB:175:GLU:CG	2.49	0.43
22:BA:1405:U:H2'	22:BA:1406:U:C6	2.53	0.43
22:BA:2899:A:H2'	22:BA:2900:A:C8	2.53	0.43
27:BF:30:ARG:H	27:BF:159:THR:HB	1.82	0.43
28:BG:42:GLU:CB	28:BG:55:ARG:HH21	2.29	0.43
45:BX:51:VAL:HG22	45:BX:52:SER:O	2.18	0.43
46:BY:49:ASP:OD1	46:BY:52:ARG:NH1	2.52	0.43
50:B2:12:ARG:CZ	50:B2:44:VAL:HG21	2.47	0.43
1:AA:4:U:O2'	1:AA:6:G:OP1	2.36	0.43
1:AA:555:U:H2'	1:AA:556:C:C6	2.53	0.43
2:AB:204:ASP:C	2:AB:205:ASP:CG	2.77	0.43
7:AG:4:ARG:HH11	7:AG:4:ARG:CG	2.31	0.43
22:BA:880:G:H2'	22:BA:881:G:C8	2.52	0.43
22:BA:2467:C:H2'	22:BA:2468:A:O4'	2.18	0.43
1:AA:323:U:H2'	1:AA:324:G:O4'	2.18	0.43
22:BA:1889:A:H2'	22:BA:1890:A:C8	2.54	0.43
35:BN:53:THR:HA	35:BN:56:LYS:HD3	2.01	0.43
8:AH:75:ILE:HD12	8:AH:129:VAL:HG22	2.01	0.43
9:AI:31:ASN:O	9:AI:33:ARG:HD2	2.18	0.43
14:AN:11:LYS:HB3	14:AN:11:LYS:HE3	1.78	0.43
19:AS:17:LYS:O	19:AS:20:GLU:HG3	2.18	0.43
22:BA:127:A:H5"	22:BA:128:C:O4'	2.18	0.43
22:BA:632:A:H2'	22:BA:633:A:C8	2.54	0.43
22:BA:1271:G:N7	22:BA:1325:U:H5	2.16	0.43
22:BA:1486:U:H2'	22:BA:1487:U:C6	2.54	0.43
22:BA:2099:U:C2'	22:BA:2100:G:O5'	2.66	0.43
22:BA:2134:A:H8	22:BA:2157:G:H21	1.66	0.43
25:BD:16:THR:HG22	25:BD:18:ASP:N	2.29	0.43
27:BF:38:MET:SD	27:BF:150:ARG:HD3	2.58	0.43
52:B4:25:VAL:HB	52:B4:35:GLN:HB2	2.01	0.43
7:AG:111:ARG:NH1	7:AG:123:GLU:N	2.66	0.43
22:BA:1484:U:H2'	22:BA:1485:U:H6	1.84	0.43
22:BA:1819:A:H5"	24:BC:160:THR:HG21	2.01	0.43
22:BA:2133:G:H2'	22:BA:2157:G:H22	1.83	0.43
22:BA:2316:G:H2'	22:BA:2317:A:C8	2.52	0.43
29:BH:15:LEU:H	29:BH:15:LEU:CD2	2.29	0.43
33:BL:19:LEU:HD22	33:BL:27:LEU:HD22	2.00	0.43
36:BO:88:LYS:HG2	36:BO:116:GLN:HG2	2.00	0.43
1:AA:974:A:OP1	14:AN:69:ARG:NH2	2.48	0.43
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.84	0.43
22:BA:1079:C:H2'	22:BA:1080:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1526:C:H2'	22:BA:1527:G:O4'	2.18	0.43
22:BA:2030:6MZ:C2	22:BA:2499:C:H5"	2.49	0.43
22:BA:2285:C:P	49:B1:6:ARG:HH21	2.42	0.43
32:BK:105:ARG:HG2	32:BK:108:ARG:HE	1.84	0.43
33:BL:29:LYS:O	33:BL:29:LYS:HG2	2.19	0.43
1:AA:976:G:OP2	1:AA:1358:U:O2'	2.37	0.43
1:AA:1148:U:H2'	1:AA:1149:C:O4'	2.19	0.43
1:AA:1226:C:H6	13:AM:102:THR:HG23	1.83	0.43
7:AG:76:LYS:HD3	7:AG:89:VAL:HG11	2.01	0.43
8:AH:96:MET:HG3	8:AH:99:LEU:HB2	2.01	0.43
9:AI:107:ASP:OD1	9:AI:109:ARG:HG3	2.19	0.43
22:BA:2455:G:H2'	22:BA:2456:C:H6	1.84	0.43
22:BA:2801:G:H2'	22:BA:2802:G:C8	2.54	0.43
44:BW:72:LYS:HE2	44:BW:72:LYS:HB2	1.88	0.43
1:AA:269:C:H2'	1:AA:270:A:H8	1.81	0.43
1:AA:383:A:O5'	1:AA:383:A:H8	2.02	0.43
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	2.01	0.43
4:AD:83:LYS:HD3	4:AD:83:LYS:N	2.34	0.43
12:AL:49:LEU:HD23	12:AL:49:LEU:HA	1.88	0.43
19:AS:19:VAL:O	19:AS:23:VAL:HG13	2.19	0.43
19:AS:36:ARG:HD2	19:AS:52:HIS:O	2.18	0.43
22:BA:881:G:H2'	22:BA:882:G:H8	1.84	0.43
22:BA:2100:G:C6	22:BA:2190:G:C2	3.07	0.43
31:BJ:95:ARG:HD2	31:BJ:96:ARG:HH11	1.83	0.43
34:BM:74:THR:HG21	34:BM:86:LYS:HE3	2.01	0.43
1:AA:110:C:O2'	16:AP:25:ARG:O	2.36	0.43
1:AA:860:A:H2'	1:AA:861:G:O4'	2.19	0.43
16:AP:42:ILE:H	16:AP:42:ILE:HG13	1.70	0.43
22:BA:1301:A:O2'	22:BA:1302:A:H3'	2.19	0.43
22:BA:1666:G:OP1	32:BK:66:LYS:HE3	2.19	0.43
28:BG:54:PRO:HG3	28:BG:62:TRP:CE2	2.54	0.43
37:BP:34:GLU:OE2	37:BP:39:ARG:NH2	2.50	0.43
1:AA:78:A:H2'	1:AA:79:G:C8	2.53	0.42
1:AA:554:A:H2'	1:AA:555:U:C6	2.54	0.42
1:AA:657:U:H4'	15:AO:28:GLN:HG2	2.01	0.42
1:AA:875:U:O2'	8:AH:15:ARG:NH1	2.50	0.42
1:AA:1119:C:H2'	1:AA:1120:C:H6	1.83	0.42
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.53	0.42
2:AB:133:GLU:HB3	2:AB:137:ARG:CD	2.47	0.42
8:AH:111:MET:HG3	8:AH:112:THR:O	2.18	0.42
22:BA:993:G:OP2	38:BQ:51:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2343:U:HO2'	22:BA:2373:G:HO2'	1.52	0.42
27:BF:112:ARG:HB3	27:BF:112:ARG:NH1	2.34	0.42
44:BW:41:ARG:HD3	44:BW:41:ARG:HA	1.82	0.42
1:AA:273:U:H1'	17:AQ:18:GLU:OE2	2.19	0.42
1:AA:559:A:H4'	1:AA:560:A:H3'	2.00	0.42
2:AB:101:LEU:HB3	2:AB:179:LEU:HD12	2.01	0.42
3:AC:156:ARG:HE	3:AC:193:TYR:HB3	1.84	0.42
5:AE:82:GLN:HB2	5:AE:83:HIS:CD2	2.52	0.42
9:AI:95:ARG:O	9:AI:99:ARG:HG2	2.19	0.42
22:BA:2150:C:H2'	22:BA:2151:U:O4'	2.19	0.42
22:BA:2799:A:O2'	22:BA:2800:A:H5"	2.20	0.42
24:BC:71:LYS:HG2	24:BC:74:ILE:HD12	2.01	0.42
28:BG:173:GLU:OE2	28:BG:176:LYS:HE2	2.19	0.42
1:AA:909:A:H5"	12:AL:18:LYS:HZ2	1.84	0.42
1:AA:1071:C:H2'	1:AA:1072:G:H8	1.84	0.42
1:AA:1095:U:H2'	1:AA:1096:C:C6	2.54	0.42
2:AB:24:ASN:ND2	2:AB:192:ASP:HB3	2.33	0.42
2:AB:139:ARG:HD2	2:AB:139:ARG:HA	1.90	0.42
2:AB:151:ILE:HG13	2:AB:154:MET:CE	2.49	0.42
22:BA:477:A:H2'	22:BA:478:A:C8	2.53	0.42
22:BA:720:U:H2'	22:BA:721:A:H8	1.84	0.42
22:BA:1198:U:H2'	22:BA:1199:U:C6	2.55	0.42
22:BA:2175:C:H2'	22:BA:2176:A:C8	2.54	0.42
22:BA:2504:PSU:N1	60:BA:3459:HOH:O	2.37	0.42
29:BH:23:ALA:O	29:BH:27:ARG:HD2	2.19	0.42
44:BW:25:ARG:HH11	44:BW:31:VAL:HG12	1.85	0.42
55:B8:37:1MG:H2'	55:B8:38:A:H8	1.84	0.42
1:AA:1022:A:H2'	1:AA:1023:U:O4'	2.20	0.42
1:AA:1478:U:H2'	1:AA:1479:C:C6	2.54	0.42
2:AB:101:LEU:N	2:AB:175:GLU:OE2	2.48	0.42
2:AB:135:LEU:HD22	2:AB:136:MET:SD	2.59	0.42
12:AL:114:ARG:HB2	12:AL:119:VAL:HB	2.00	0.42
15:AO:8:THR:HG23	15:AO:31:LEU:HD21	2.01	0.42
22:BA:1637:A:H5'	22:BA:1760:C:O2'	2.19	0.42
55:B8:20:U:H6	55:B8:20:U:H2'	1.63	0.42
1:AA:89:U:H2'	1:AA:90:C:H6	1.85	0.42
1:AA:160:A:H2'	1:AA:161:A:O4'	2.19	0.42
1:AA:975:A:H8	1:AA:1357:A:HO2'	1.66	0.42
1:AA:1038:C:H2'	1:AA:1039:G:C8	2.52	0.42
1:AA:1118:U:H2'	1:AA:1119:C:H6	1.84	0.42
5:AE:86:LYS:HD2	5:AE:94:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:70:LEU:HD12	15:AO:70:LEU:O	2.19	0.42
22:BA:568:U:OP1	33:BL:36:LYS:HE2	2.19	0.42
4:AD:161:LEU:HD23	4:AD:161:LEU:HA	1.88	0.42
15:AO:36:ILE:HG13	15:AO:59:MET:CE	2.49	0.42
15:AO:36:ILE:HG13	15:AO:59:MET:HE2	2.00	0.42
22:BA:483:A:OP1	42:BU:47:LYS:HE2	2.19	0.42
22:BA:687:C:H1'	50:B2:4:THR:HG22	2.01	0.42
22:BA:848:C:H2'	22:BA:849:A:H8	1.84	0.42
28:BG:149:ARG:HA	28:BG:162:VAL:HG13	2.00	0.42
32:BK:106:GLU:OE1	32:BK:106:GLU:N	2.52	0.42
1:AA:426:U:P	4:AD:33:LYS:HZ1	2.41	0.42
1:AA:1013:G:N2	1:AA:1016:A:OP2	2.49	0.42
13:AM:39:ILE:HG22	13:AM:40:ALA:O	2.20	0.42
22:BA:1545:A:H2'	22:BA:1546:G:O4'	2.20	0.42
29:BH:87:GLU:OE1	29:BH:89:LYS:HB3	2.20	0.42
39:BR:58:VAL:HG12	39:BR:60:LYS:CD	2.50	0.42
48:B0:43:ILE:HG22	48:B0:49:TYR:HB2	2.00	0.42
1:AA:736:C:H2'	1:AA:737:C:C6	2.54	0.42
2:AB:179:LEU:HD23	2:AB:179:LEU:HA	1.90	0.42
5:AE:105:ILE:O	5:AE:112:ARG:NH1	2.44	0.42
22:BA:1182:G:H2'	22:BA:1183:U:O4'	2.19	0.42
22:BA:1438:U:H2'	22:BA:1439:A:H8	1.85	0.42
27:BF:126:GLY:O	27:BF:158:THR:OG1	2.30	0.42
29:BH:15:LEU:HD21	29:BH:58:LEU:HD22	2.02	0.42
34:BM:75:GLU:HG3	34:BM:90:GLU:CG	2.50	0.42
2:AB:108:ARG:O	2:AB:111:ILE:HG12	2.20	0.42
2:AB:132:LYS:HB2	2:AB:133:GLU:HG2	2.01	0.42
4:AD:56:ARG:HH21	4:AD:59:GLN:HG3	1.83	0.42
13:AM:74:SER:O	13:AM:78:LYS:HG3	2.20	0.42
22:BA:367:G:H2'	22:BA:368:A:C8	2.55	0.42
22:BA:1039:A:H2	22:BA:1116:G:H22	1.68	0.42
22:BA:1585:C:H2'	22:BA:1586:A:O4'	2.19	0.42
22:BA:2687:U:H2'	22:BA:2688:G:O4'	2.20	0.42
30:BI:8:LYS:HA	30:BI:8:LYS:HD2	1.83	0.42
1:AA:190:A:O5'	1:AA:190:A:H8	2.03	0.42
1:AA:1397:C:P	5:AE:29:ARG:HH22	2.43	0.42
1:AA:1477:U:H2'	1:AA:1478:U:C6	2.55	0.42
2:AB:117:LEU:CD1	2:AB:141:LEU:HG	2.50	0.42
9:AI:44:ALA:O	9:AI:48:VAL:HG23	2.19	0.42
19:AS:33:THR:HG23	19:AS:51:VAL:HA	2.01	0.42
22:BA:657:U:H2'	22:BA:658:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1797:G:O2'	24:BC:257:THR:OG1	2.20	0.42
22:BA:2547:A:H2'	22:BA:2548:U:C6	2.54	0.42
26:BE:192:ALA:O	26:BE:196:VAL:HG13	2.20	0.42
1:AA:1027:C:H2'	1:AA:1028:C:C6	2.55	0.41
5:AE:83:HIS:HE1	5:AE:85:VAL:HG12	1.82	0.41
6:AF:102:MET:CE	18:AR:24:LYS:HB3	2.50	0.41
9:AI:44:ALA:O	9:AI:47:VAL:HG22	2.19	0.41
22:BA:1680:U:H2'	22:BA:1681:G:O4'	2.20	0.41
22:BA:1872:A:H2'	22:BA:1873:G:O4'	2.20	0.41
24:BC:181:MET:HB2	24:BC:268:VAL:HB	2.02	0.41
29:BH:108:VAL:HG13	29:BH:109:GLU:N	2.33	0.41
31:BJ:35:ARG:HB2	31:BJ:54:ILE:HD11	2.02	0.41
35:BN:49:GLU:O	35:BN:53:THR:HG23	2.20	0.41
49:B1:11:LEU:HB3	49:B1:49:TYR:HB3	2.01	0.41
1:AA:462:G:H2'	1:AA:463:U:C6	2.55	0.41
1:AA:1279:G:P	10:AJ:9:ARG:NH2	2.93	0.41
1:AA:1507:A:H2'	1:AA:1508:A:C8	2.55	0.41
2:AB:18:HIS:CD2	2:AB:188:ASP:CG	2.94	0.41
3:AC:72:ARG:HD3	3:AC:72:ARG:HA	1.91	0.41
4:AD:104:ARG:HG2	4:AD:104:ARG:NH1	2.35	0.41
22:BA:746:PSU:H2'	60:BA:4751:HOH:O	2.19	0.41
22:BA:2243:U:H2'	22:BA:2244:U:C6	2.55	0.41
22:BA:2484:G:OP1	34:BM:44:ARG:NH1	2.46	0.41
26:BE:23:PHE:HA	26:BE:107:SER:OG	2.20	0.41
27:BF:110:ARG:HE	27:BF:110:ARG:HB3	1.65	0.41
28:BG:141:ILE:HD12	28:BG:141:ILE:HA	1.93	0.41
43:BV:63:ILE:HG22	43:BV:65:VAL:HG23	2.02	0.41
1:AA:467:U:H3'	1:AA:468:A:C5'	2.51	0.41
1:AA:1530:G:H2'	1:AA:1531:A:H8	1.85	0.41
9:AI:54:LEU:HD13	9:AI:97:GLU:OE2	2.20	0.41
14:AN:15:LEU:HD23	14:AN:55:SER:HB3	2.02	0.41
22:BA:282:A:H2'	22:BA:283:G:C8	2.56	0.41
22:BA:1645:G:H5"	22:BA:1646:C:H5'	2.03	0.41
22:BA:1820:U:OP1	24:BC:177:ARG:NE	2.53	0.41
27:BF:103:LEU:HA	27:BF:107:ALA:HB3	2.02	0.41
36:BO:49:VAL:HG21	36:BO:81:ARG:HB2	2.02	0.41
40:BS:68:ASP:OD1	40:BS:68:ASP:N	2.52	0.41
1:AA:162:A:O5'	1:AA:162:A:H8	2.02	0.41
1:AA:514:C:C2	1:AA:515:G:C8	3.08	0.41
2:AB:8:ASP:OD1	2:AB:9:MET:HG3	2.20	0.41
10:AJ:41:PRO:HA	10:AJ:72:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BB:43:C:O2	27:BF:92:ARG:NH1	2.47	0.41
26:BE:153:LEU:HD21	26:BE:158:PHE:HB2	2.01	0.41
29:BH:132:PHE:CD1	29:BH:132:PHE:N	2.89	0.41
55:B8:71:C:H2'	55:B8:72:G:H8	1.83	0.41
1:AA:161:A:H2'	1:AA:162:A:C8	2.55	0.41
1:AA:722:G:N3	1:AA:722:G:H2'	2.35	0.41
1:AA:1326:U:H2'	1:AA:1327:C:H6	1.85	0.41
3:AC:9:GLY:HA3	14:AN:89:MET:HE3	2.03	0.41
3:AC:134:MET:HE2	3:AC:168:TYR:CD1	2.55	0.41
9:AI:47:VAL:HA	9:AI:50:GLN:CG	2.50	0.41
22:BA:1970:A:H5'	22:BA:1972:G:H1'	2.03	0.41
22:BA:2552:OMU:HM23	22:BA:2554:U:C6	2.55	0.41
27:BF:94:GLU:OE2	27:BF:98:GLU:CG	2.69	0.41
31:BJ:31:GLU:OE1	31:BJ:31:GLU:HA	2.20	0.41
1:AA:1495:U:H2'	1:AA:1496:C:H6	1.85	0.41
1:AA:1495:U:H2'	1:AA:1496:C:C6	2.56	0.41
13:AM:56:LEU:HA	13:AM:56:LEU:HD12	1.77	0.41
14:AN:46:LEU:HD12	14:AN:46:LEU:O	2.19	0.41
22:BA:288:U:H2'	22:BA:289:G:H8	1.86	0.41
22:BA:871:U:H2'	22:BA:872:U:H6	1.86	0.41
22:BA:1076:C:H2'	22:BA:1077:A:C8	2.56	0.41
22:BA:1930:G:N2	22:BA:1968:G:H2'	2.36	0.41
23:BB:66:A:H61	23:BB:107:G:H2'	1.86	0.41
39:BR:60:LYS:NZ	39:BR:102:SER:OG	2.53	0.41
40:BS:4:ILE:HG12	40:BS:106:VAL:HG22	2.02	0.41
1:AA:88:U:O2'	1:AA:89:U:C6	2.72	0.41
1:AA:454:G:N2	1:AA:479:U:O2	2.54	0.41
1:AA:864:A:H2'	1:AA:865:A:C8	2.55	0.41
1:AA:1005:A:C4	1:AA:1006:G:C8	3.08	0.41
5:AE:111:MET:HE1	5:AE:125:ALA:HB1	2.01	0.41
10:AJ:65:TYR:OH	14:AN:85:ARG:HG3	2.21	0.41
22:BA:635:C:OP2	33:BL:126:ARG:NH2	2.50	0.41
22:BA:644:A:H2'	22:BA:645:C:O4'	2.21	0.41
22:BA:1563:U:H2'	22:BA:1564:C:C6	2.56	0.41
22:BA:2105:U:H2'	22:BA:2106:U:C6	2.55	0.41
33:BL:79:LEU:HD11	33:BL:112:LEU:HD12	2.03	0.41
38:BQ:86:ALA:O	39:BR:51:VAL:HG23	2.21	0.41
45:BX:6:GLN:HG3	45:BX:50:ARG:O	2.21	0.41
1:AA:1000:A:N6	1:AA:1041:G:O6	2.54	0.41
6:AF:56:LYS:HE3	6:AF:56:LYS:HB3	1.89	0.41
22:BA:1810:A:O5'	22:BA:1810:A:H8	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1853:A:H2'	22:BA:1854:A:C8	2.56	0.41
22:BA:2720:U:OP1	37:BP:53:ARG:NH2	2.54	0.41
43:BV:73:LYS:NZ	43:BV:73:LYS:HB3	2.36	0.41
1:AA:113:G:H1'	1:AA:354:G:H5'	2.03	0.41
1:AA:649:A:H2'	1:AA:650:G:O4'	2.21	0.41
7:AG:142:HIS:O	7:AG:145:ALA:N	2.54	0.41
14:AN:73:PHE:CE1	14:AN:78:GLY:HA2	2.56	0.41
19:AS:7:LYS:HZ3	19:AS:7:LYS:HG3	1.81	0.41
20:AT:76:LYS:O	20:AT:80:THR:HG23	2.21	0.41
22:BA:876:C:H2'	22:BA:877:A:O4'	2.21	0.41
22:BA:882:G:N2	22:BA:895:U:H1'	2.35	0.41
22:BA:2876:G:OP1	37:BP:2:SER:N	2.54	0.41
22:BA:2895:G:H2'	22:BA:2896:C:C6	2.56	0.41
24:BC:75:PRO:HB2	24:BC:97:LYS:HE2	2.02	0.41
33:BL:13:LYS:HD3	33:BL:13:LYS:HA	1.86	0.41
33:BL:129:LYS:HE3	33:BL:129:LYS:HB3	1.75	0.41
34:BM:77:PRO:HG2	34:BM:80:VAL:HG11	2.02	0.41
36:BO:39:VAL:HB	36:BO:49:VAL:HG13	2.03	0.41
55:B8:22:G:C5	55:B8:46:G7M:N2	2.68	0.41
55:B8:63:U:H2'	55:B8:64:C:H6	1.85	0.41
1:AA:1464:U:H2'	1:AA:1465:A:C8	2.56	0.41
3:AC:169:ARG:HD2	3:AC:170:GLU:N	2.36	0.41
4:AD:124:MET:HE3	4:AD:129:VAL:HG22	2.03	0.41
8:AH:36:ILE:HD11	8:AH:126:ILE:HG21	2.03	0.41
17:AQ:58:VAL:HG12	17:AQ:79:VAL:CG2	2.51	0.41
19:AS:32:ARG:HE	19:AS:57:HIS:CD2	2.38	0.41
20:AT:51:PHE:CE1	20:AT:55:GLN:HG3	2.56	0.41
22:BA:171:U:H2'	22:BA:172:A:H8	1.86	0.41
22:BA:288:U:H2'	22:BA:289:G:C8	2.56	0.41
22:BA:811:U:H2'	33:BL:21:ARG:HA	2.02	0.41
22:BA:1541:C:H2'	22:BA:1542:U:C6	2.56	0.41
22:BA:2014:A:H2'	22:BA:2015:A:C8	2.55	0.41
22:BA:2271:G:OP1	44:BW:18:ALA:HB1	2.21	0.41
22:BA:2300:C:H2'	22:BA:2301:C:H6	1.86	0.41
24:BC:138:GLY:O	24:BC:163:GLN:NE2	2.53	0.41
1:AA:580:C:H2'	1:AA:581:G:O4'	2.21	0.40
1:AA:677:U:H3	1:AA:713:G:H22	1.69	0.40
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.56	0.40
20:AT:24:ARG:HA	20:AT:24:ARG:HD3	1.82	0.40
22:BA:2502:G:H5"	22:BA:2503:2MA:H5"	2.02	0.40
27:BF:162:SER:OG	27:BF:164:GLU:CD	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BT:1:MET:HB2	41:BT:2:ILE:H	1.50	0.40
42:BU:85:PHE:CE1	42:BU:94:ARG:HG2	2.56	0.40
3:AC:83:ASP:OD1	3:AC:84:VAL:N	2.54	0.40
5:AE:111:MET:HE2	5:AE:125:ALA:HB1	2.03	0.40
8:AH:46:ILE:HD13	8:AH:61:LEU:HD23	2.04	0.40
9:AI:65:ILE:HD13	9:AI:79:ILE:HG23	2.03	0.40
13:AM:4:ILE:HA	13:AM:57:ARG:HG2	2.04	0.40
13:AM:78:LYS:HB2	13:AM:78:LYS:HE2	1.87	0.40
22:BA:634:C:H2'	22:BA:635:C:C6	2.57	0.40
22:BA:851:C:H2'	22:BA:852:U:C6	2.55	0.40
22:BA:1544:A:H2'	22:BA:1545:A:C8	2.56	0.40
22:BA:1914:C:H2'	22:BA:1915:3TD:H6	2.03	0.40
22:BA:2246:G:H2'	22:BA:2247:A:H8	1.85	0.40
1:AA:79:G:H2'	1:AA:80:A:C8	2.56	0.40
1:AA:95:C:O2	1:AA:95:C:H2'	2.21	0.40
1:AA:216:U:H2'	1:AA:217:C:H6	1.83	0.40
1:AA:579:A:H2'	1:AA:580:C:C6	2.56	0.40
1:AA:1041:G:H2'	1:AA:1042:A:C8	2.55	0.40
1:AA:1329:A:H5"	13:AM:26:GLY:H	1.85	0.40
3:AC:42:TYR:CD1	3:AC:43:LEU:HD12	2.54	0.40
5:AE:148:ASN:OD1	8:AH:96:MET:CE	2.70	0.40
22:BA:347:A:H2'	22:BA:348:A:H8	1.86	0.40
22:BA:1051:G:H2'	22:BA:1052:C:O4'	2.21	0.40
22:BA:1790:C:H2'	22:BA:1791:A:C5	2.56	0.40
22:BA:2020:A:H5'	48:B0:9:THR:CG2	2.50	0.40
22:BA:2615:U:C2	48:B0:4:GLN:HA	2.56	0.40
49:B1:13:SER:HB2	49:B1:49:TYR:CZ	2.56	0.40
55:B8:28:U:H2'	55:B8:29:U:H6	1.87	0.40
1:AA:182:A:C4	1:AA:184:G:C8	3.10	0.40
1:AA:672:U:H2'	1:AA:673:A:H8	1.86	0.40
1:AA:696:A:H2'	1:AA:697:U:C6	2.55	0.40
1:AA:952:U:O4	13:AM:103:LYS:HD3	2.21	0.40
3:AC:88:ARG:HB3	3:AC:101:ILE:HG13	2.03	0.40
5:AE:55:GLU:OE1	5:AE:55:GLU:HA	2.21	0.40
13:AM:3:ARG:HH22	13:AM:7:ILE:HG23	1.86	0.40
17:AQ:39:LYS:NZ	17:AQ:39:LYS:O	2.47	0.40
19:AS:19:VAL:CG2	19:AS:44:MET:HB3	2.51	0.40
22:BA:2305:U:H2'	22:BA:2306:C:C6	2.57	0.40
26:BE:69:ARG:H	26:BE:69:ARG:HG2	1.62	0.40
29:BH:82:SER:HB2	29:BH:90:LEU:HD13	2.04	0.40
1:AA:222:C:H2'	1:AA:223:A:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:235:C:H2'	1:AA:236:A:H8	1.84	0.40
1:AA:399:G:H2'	1:AA:400:C:C6	2.57	0.40
1:AA:1012:A:C6	1:AA:1018:G:C6	3.09	0.40
2:AB:102:THR:HG23	2:AB:175:GLU:HG3	2.02	0.40
7:AG:42:ILE:HD12	7:AG:116:MET:HB3	2.03	0.40
9:AI:55:VAL:HG22	9:AI:94:LEU:HD22	2.04	0.40
16:AP:71:VAL:O	16:AP:75:ILE:HG13	2.20	0.40
22:BA:576:U:H2'	22:BA:577:G:C8	2.56	0.40
22:BA:2151:U:H2'	22:BA:2152:G:H8	1.86	0.40
23:BB:106:G:H2'	23:BB:107:G:O4'	2.22	0.40
27:BF:71:ARG:O	27:BF:81:GLN:HG3	2.22	0.40
30:BI:14:ALA:N	30:BI:22:MET:O	2.55	0.40
36:BO:33:ARG:O	36:BO:65:THR:OG1	2.39	0.40
55:B8:65:U:H2'	55:B8:66:A:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/240 (92%)	211 (95%)	11 (5%)	0	100	100
3	AC	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
4	AD	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
5	AE	153/167 (92%)	146 (95%)	7 (5%)	0	100	100
6	AF	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	AG	149/179 (83%)	136 (91%)	13 (9%)	0	100	100
8	AH	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	AI	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
10	AJ	97/103 (94%)	92 (95%)	4 (4%)	1 (1%)	15	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	AL	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	AM	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
14	AN	99/102 (97%)	91 (92%)	8 (8%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
17	AQ	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	80/92 (87%)	74 (92%)	6 (8%)	0	100	100
20	AT	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
25	BD	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
26	BE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	BF	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
28	BG	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
33	BL	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
34	BM	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
35	BN	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
36	BO	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
37	BP	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
40	BS	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
41	BT	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
42	BU	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
43	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BW	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	BX	75/78 (96%)	75 (100%)	0	0	100	100
46	BY	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	BZ	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	B0	54/57 (95%)	54 (100%)	0	0	100	100
49	B1	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
50	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	B3	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	B5	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
All	All	5590/5930 (94%)	5381 (96%)	208 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	AJ	57	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/198 (94%)	182 (98%)	4 (2%)	52	71
3	AC	170/190 (90%)	163 (96%)	7 (4%)	30	48
4	AD	172/173 (99%)	167 (97%)	5 (3%)	42	62
5	AE	118/126 (94%)	115 (98%)	3 (2%)	47	67
6	AF	92/116 (79%)	91 (99%)	1 (1%)	73	87
7	AG	124/147 (84%)	115 (93%)	9 (7%)	14	22
8	AH	104/105 (99%)	101 (97%)	3 (3%)	42	62
9	AI	105/107 (98%)	101 (96%)	4 (4%)	33	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	AJ	87/90 (97%)	82 (94%)	5 (6%)	20 33
11	AK	90/99 (91%)	89 (99%)	1 (1%)	73 87
12	AL	102/103 (99%)	97 (95%)	5 (5%)	25 40
13	AM	92/96 (96%)	92 (100%)	0	100 100
14	AN	79/84 (94%)	76 (96%)	3 (4%)	33 51
15	AO	76/77 (99%)	74 (97%)	2 (3%)	46 66
16	AP	65/65 (100%)	65 (100%)	0	100 100
17	AQ	74/78 (95%)	72 (97%)	2 (3%)	44 65
18	AR	48/65 (74%)	46 (96%)	2 (4%)	30 47
19	AS	71/79 (90%)	70 (99%)	1 (1%)	67 82
20	AT	65/66 (98%)	65 (100%)	0	100 100
21	AU	48/61 (79%)	45 (94%)	3 (6%)	18 28
24	BC	216/218 (99%)	213 (99%)	3 (1%)	67 82
25	BD	163/163 (100%)	157 (96%)	6 (4%)	34 53
26	BE	165/165 (100%)	162 (98%)	3 (2%)	59 76
27	BF	148/150 (99%)	142 (96%)	6 (4%)	30 48
28	BG	137/138 (99%)	134 (98%)	3 (2%)	52 71
29	BH	114/114 (100%)	112 (98%)	2 (2%)	59 76
30	BI	59/62 (95%)	57 (97%)	2 (3%)	37 56
31	BJ	116/116 (100%)	114 (98%)	2 (2%)	60 78
32	BK	104/104 (100%)	101 (97%)	3 (3%)	42 62
33	BL	103/103 (100%)	102 (99%)	1 (1%)	76 88
34	BM	108/108 (100%)	104 (96%)	4 (4%)	34 53
35	BN	98/103 (95%)	98 (100%)	0	100 100
36	BO	87/87 (100%)	84 (97%)	3 (3%)	37 56
37	BP	99/100 (99%)	96 (97%)	3 (3%)	41 61
38	BQ	89/90 (99%)	88 (99%)	1 (1%)	73 87
39	BR	84/84 (100%)	82 (98%)	2 (2%)	49 68
40	BS	93/93 (100%)	93 (100%)	0	100 100
41	BT	80/84 (95%)	78 (98%)	2 (2%)	47 67
42	BU	83/85 (98%)	82 (99%)	1 (1%)	71 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BV	78/78 (100%)	76 (97%)	2 (3%)	46	66
44	BW	57/63 (90%)	55 (96%)	2 (4%)	36	55
45	BX	67/68 (98%)	66 (98%)	1 (2%)	65	80
46	BY	54/55 (98%)	53 (98%)	1 (2%)	57	75
47	BZ	48/49 (98%)	47 (98%)	1 (2%)	53	72
48	B0	47/48 (98%)	44 (94%)	3 (6%)	17	28
49	B1	45/49 (92%)	44 (98%)	1 (2%)	52	71
50	B2	38/38 (100%)	36 (95%)	2 (5%)	22	37
51	B3	51/52 (98%)	50 (98%)	1 (2%)	55	74
52	B4	34/34 (100%)	33 (97%)	1 (3%)	42	62
53	B5	17/17 (100%)	16 (94%)	1 (6%)	19	32
All	All	4650/4843 (96%)	4527 (97%)	123 (3%)	49	66

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	21	ARG
2	AB	69	PHE
2	AB	91	PHE
2	AB	136	MET
3	AC	59	ARG
3	AC	88	ARG
3	AC	122	SER
3	AC	129	MET
3	AC	139	GLN
3	AC	170	GLU
3	AC	186	THR
4	AD	8	LYS
4	AD	56	ARG
4	AD	63	ARG
4	AD	78	GLU
4	AD	124	MET
5	AE	54	ARG
5	AE	66	LYS
5	AE	93	ARG
6	AF	45	ARG
7	AG	3	ARG
7	AG	11	LYS

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Mol	Chain	Res	Type
7	AG	28	ASN
7	AG	41	SER
7	AG	79	ARG
7	AG	95	ARG
7	AG	113	ASP
7	AG	130	ASN
7	AG	131	LYS
8	AH	50	LYS
8	AH	89	LYS
8	AH	117	ARG
9	AI	4	ASN
9	AI	12	ARG
9	AI	60	LYS
9	AI	106	ARG
10	AJ	17	LEU
10	AJ	63	ASP
10	AJ	72	ARG
10	AJ	99	GLN
10	AJ	101	SER
11	AK	26	SER
12	AL	45	PRO
12	AL	47	SER
12	AL	51	LYS
12	AL	78	SER
12	AL	111	LYS
14	AN	4	SER
14	AN	63	ARG
14	AN	69	ARG
15	AO	24	SER
15	AO	58	ARG
17	AQ	39	LYS
17	AQ	77	ARG
18	AR	61	ARG
18	AR	73	ARG
19	AS	44	MET
21	AU	25	LYS
21	AU	35	ARG
21	AU	47	ARG
24	BC	5	LYS
24	BC	182	ARG
24	BC	270	ARG
25	BD	7	LYS

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Mol	Chain	Res	Type
25	BD	13	ARG
25	BD	39	ASP
25	BD	100	LEU
25	BD	113	SER
25	BD	181	ASP
26	BE	88	ARG
26	BE	93	SER
26	BE	168	ASP
27	BF	51	ASP
27	BF	73	SER
27	BF	80	ARG
27	BF	127	ASN
27	BF	133	ARG
27	BF	162	SER
28	BG	69	ARG
28	BG	86	LYS
28	BG	175	LYS
29	BH	51	ARG
29	BH	97	ARG
30	BI	3	LYS
30	BI	15	SER
31	BJ	1	MET
31	BJ	95	ARG
32	BK	51	LYS
32	BK	53	LYS
32	BK	117	SER
33	BL	129	LYS
34	BM	6	ARG
34	BM	55	ARG
34	BM	115	GLU
34	BM	127	LYS
36	BO	1	MET
36	BO	45	SER
36	BO	63	LYS
37	BP	19	SER
37	BP	65	SER
37	BP	89	ARG
38	BQ	84	LYS
39	BR	18	GLN
39	BR	85	LYS
41	BT	24	MET
41	BT	64	LYS

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Mol	Chain	Res	Type
42	BU	81	ASP
43	BV	58	SER
43	BV	71	LYS
44	BW	44	LYS
44	BW	81	SER
45	BX	72	ARG
46	BY	23	ARG
47	BZ	39	GLU
48	B0	11	SER
48	B0	52	ARG
48	B0	53	LYS
49	B1	10	LYS
50	B2	25	LYS
50	B2	41	ARG
51	B3	31	HIS
52	B4	20	ASP
53	B5	24	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
5	AE	135	ASN
9	AI	50	GLN
19	AS	57	HIS
28	BG	38	ASN
50	B2	26	ASN
50	B2	29	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	180 (11%)	1 (0%)
22	BA	2891/2897 (99%)	295 (10%)	15 (0%)
23	BB	119/120 (99%)	7 (5%)	0
54	B7	8/9 (88%)	4 (50%)	0
55	B8	76/77 (98%)	14 (18%)	4 (5%)
All	All	4624/4637 (99%)	500 (10%)	20 (0%)

All (500) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	22	G
1	AA	39	G
1	AA	44	A
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	71	A
1	AA	72	A
1	AA	76	G
1	AA	78	A
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	87	C
1	AA	88	U
1	AA	89	U
1	AA	95	C
1	AA	98	A
1	AA	101	A
1	AA	116	A
1	AA	130	A
1	AA	131	A
1	AA	163	C
1	AA	164	G
1	AA	167	A
1	AA	181	A
1	AA	197	A
1	AA	210	C
1	AA	226	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	306	A
1	AA	321	A
1	AA	328	C

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Mol	Chain	Res	Type
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	384	G
1	AA	392	C
1	AA	393	A
1	AA	397	A
1	AA	398	U
1	AA	406	G
1	AA	408	A
1	AA	413	G
1	AA	429	U
1	AA	435	A
1	AA	437	U
1	AA	439	U
1	AA	467	U
1	AA	468	A
1	AA	478	A
1	AA	479	U
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	488	C
1	AA	497	G
1	AA	509	A
1	AA	511	C
1	AA	513	C
1	AA	516	PSU
1	AA	518	C
1	AA	527	G7M
1	AA	532	A
1	AA	547	A
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	617	G
1	AA	633	G
1	AA	650	G

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Mol	Chain	Res	Type
1	AA	653	U
1	AA	665	A
1	AA	702	A
1	AA	718	A
1	AA	721	G
1	AA	722	G
1	AA	724	G
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	815	A
1	AA	817	C
1	AA	828	U
1	AA	832	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	846	G
1	AA	914	A
1	AA	926	G
1	AA	934	C
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	993	G
1	AA	1004	A
1	AA	1005	A
1	AA	1012	A
1	AA	1016	A
1	AA	1019	A
1	AA	1020	G
1	AA	1021	A
1	AA	1026	G
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U

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Mol	Chain	Res	Type
1	AA	1032	G
1	AA	1045	C
1	AA	1053	G
1	AA	1065	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1132	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1157	A
1	AA	1158	C
1	AA	1159	U
1	AA	1168	U
1	AA	1169	A
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1212	U
1	AA	1213	A
1	AA	1227	A
1	AA	1238	A
1	AA	1256	A
1	AA	1258	G
1	AA	1260	G
1	AA	1280	A
1	AA	1285	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C
1	AA	1317	C
1	AA	1318	A
1	AA	1320	C
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1364	U
1	AA	1370	G
1	AA	1419	G
1	AA	1429	A
1	AA	1441	A

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Mol	Chain	Res	Type
1	AA	1446	A
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1497	G
1	AA	1499	A
1	AA	1502	A
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
22	BA	34	U
22	BA	61	C
22	BA	71	A
22	BA	74	A
22	BA	75	G
22	BA	84	A
22	BA	101	A
22	BA	118	A
22	BA	119	A
22	BA	120	U
22	BA	163	C
22	BA	181	A
22	BA	196	A
22	BA	215	G
22	BA	216	A
22	BA	221	A
22	BA	222	A
22	BA	233	A
22	BA	248	G
22	BA	265	A
22	BA	276	U
22	BA	278	A
22	BA	302	C
22	BA	303	G
22	BA	311	A
22	BA	330	A
22	BA	353	C
22	BA	386	G
22	BA	396	G
22	BA	411	G
22	BA	412	A

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Mol	Chain	Res	Type
22	BA	480	A
22	BA	481	G
22	BA	491	G
22	BA	505	A
22	BA	509	C
22	BA	529	A
22	BA	530	G
22	BA	531	C
22	BA	532	A
22	BA	544	C
22	BA	546	U
22	BA	547	A
22	BA	548	G
22	BA	549	G
22	BA	563	A
22	BA	573	U
22	BA	575	A
22	BA	603	A
22	BA	614	A
22	BA	637	A
22	BA	645	C
22	BA	647	G
22	BA	654	A
22	BA	655	A
22	BA	685	A
22	BA	686	U
22	BA	717	C
22	BA	730	A
22	BA	738	G
22	BA	747	5MU
22	BA	764	A
22	BA	765	C
22	BA	775	G
22	BA	776	G
22	BA	782	A
22	BA	784	G
22	BA	785	G
22	BA	789	A
22	BA	792	A
22	BA	805	G
22	BA	812	C
22	BA	827	U

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Mol	Chain	Res	Type
22	BA	828	U
22	BA	829	A
22	BA	846	U
22	BA	847	U
22	BA	858	G
22	BA	859	G
22	BA	884	U
22	BA	896	A
22	BA	910	A
22	BA	931	U
22	BA	946	C
22	BA	961	C
22	BA	974	G
22	BA	983	A
22	BA	996	A
22	BA	1012	U
22	BA	1013	C
22	BA	1026	G
22	BA	1033	U
22	BA	1054	A
22	BA	1070	A
22	BA	1088	A
22	BA	1112	G
22	BA	1132	U
22	BA	1133	A
22	BA	1135	C
22	BA	1142	A
22	BA	1173	U
22	BA	1174	U
22	BA	1175	A
22	BA	1176	U
22	BA	1204	A
22	BA	1250	G
22	BA	1253	A
22	BA	1256	G
22	BA	1268	A
22	BA	1271	G
22	BA	1272	A
22	BA	1273	U
22	BA	1287	A
22	BA	1300	G
22	BA	1301	A

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Mol	Chain	Res	Type
22	BA	1321	A
22	BA	1329	U
22	BA	1352	U
22	BA	1365	A
22	BA	1379	U
22	BA	1383	A
22	BA	1416	G
22	BA	1420	A
22	BA	1428	C
22	BA	1452	G
22	BA	1482	G
22	BA	1508	A
22	BA	1509	A
22	BA	1515	A
22	BA	1566	A
22	BA	1569	A
22	BA	1578	U
22	BA	1606	C
22	BA	1608	A
22	BA	1610	A
22	BA	1647	U
22	BA	1648	U
22	BA	1649	G
22	BA	1674	G
22	BA	1677	A
22	BA	1729	U
22	BA	1730	C
22	BA	1732	C
22	BA	1757	A
22	BA	1758	U
22	BA	1764	C
22	BA	1773	A
22	BA	1782	U
22	BA	1800	C
22	BA	1801	A
22	BA	1802	A
22	BA	1808	A
22	BA	1811	G
22	BA	1816	C
22	BA	1829	A
22	BA	1871	A
22	BA	1872	A

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Mol	Chain	Res	Type
22	BA	1873	G
22	BA	1906	G
22	BA	1914	C
22	BA	1929	G
22	BA	1930	G
22	BA	1937	A
22	BA	1938	A
22	BA	1955	U
22	BA	1960	A
22	BA	1967	C
22	BA	1970	A
22	BA	1971	U
22	BA	1972	G
22	BA	1991	U
22	BA	1993	U
22	BA	2020	A
22	BA	2023	C
22	BA	2027	G
22	BA	2031	A
22	BA	2033	A
22	BA	2036	C
22	BA	2043	C
22	BA	2055	C
22	BA	2056	G
22	BA	2060	A
22	BA	2061	G
22	BA	2062	A
22	BA	2069	G7M
22	BA	2080	A
22	BA	2099	U
22	BA	2101	A
22	BA	2110	G
22	BA	2111	U
22	BA	2112	G
22	BA	2113	U
22	BA	2115	G
22	BA	2116	G
22	BA	2117	A
22	BA	2118	U
22	BA	2119	A
22	BA	2124	G
22	BA	2125	G

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Mol	Chain	Res	Type
22	BA	2126	A
22	BA	2127	G
22	BA	2128	G
22	BA	2131	U
22	BA	2132	U
22	BA	2133	G
22	BA	2137	U
22	BA	2142	A
22	BA	2147	A
22	BA	2157	G
22	BA	2158	A
22	BA	2159	G
22	BA	2163	A
22	BA	2164	C
22	BA	2165	C
22	BA	2171	A
22	BA	2172	U
22	BA	2173	A
22	BA	2182	U
22	BA	2183	A
22	BA	2188	U
22	BA	2189	U
22	BA	2190	G
22	BA	2195	U
22	BA	2198	A
22	BA	2204	G
22	BA	2211	A
22	BA	2225	A
22	BA	2238	G
22	BA	2239	G
22	BA	2252	G
22	BA	2278	A
22	BA	2283	C
22	BA	2287	A
22	BA	2288	A
22	BA	2305	U
22	BA	2308	G
22	BA	2322	A
22	BA	2325	G
22	BA	2333	A
22	BA	2336	A
22	BA	2345	G

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Mol	Chain	Res	Type
22	BA	2347	C
22	BA	2350	C
22	BA	2368	C
22	BA	2383	G
22	BA	2385	C
22	BA	2402	U
22	BA	2406	A
22	BA	2425	A
22	BA	2429	G
22	BA	2430	A
22	BA	2435	A
22	BA	2441	U
22	BA	2448	A
22	BA	2476	A
22	BA	2478	A
22	BA	2491	U
22	BA	2502	G
22	BA	2504	PSU
22	BA	2505	G
22	BA	2518	A
22	BA	2529	G
22	BA	2535	G
22	BA	2547	A
22	BA	2566	A
22	BA	2567	G
22	BA	2602	A
22	BA	2609	U
22	BA	2613	U
22	BA	2615	U
22	BA	2629	U
22	BA	2630	G
22	BA	2663	G
22	BA	2682	A
22	BA	2689	U
22	BA	2690	U
22	BA	2714	G
22	BA	2716	C
22	BA	2726	A
22	BA	2733	A
22	BA	2744	G
22	BA	2748	A
22	BA	2778	A

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Mol	Chain	Res	Type
22	BA	2791	G
22	BA	2820	A
22	BA	2821	A
22	BA	2835	A
22	BA	2861	U
22	BA	2873	A
22	BA	2874	C
22	BA	2880	C
22	BA	2883	A
22	BA	2884	U
22	BA	2885	G
22	BA	2891	U
23	BB	35	C
23	BB	44	G
23	BB	56	G
23	BB	89	U
23	BB	90	C
23	BB	105	G
23	BB	109	A
54	B7	4	C
54	B7	7	U
54	B7	8	G
54	B7	9	A
55	B8	3	G
55	B8	4	U
55	B8	5	G
55	B8	6	A
55	B8	14	A
55	B8	17	C
55	B8	19	G
55	B8	20	U
55	B8	21	A
55	B8	22	G
55	B8	36	G
55	B8	46	G7M
55	B8	47	U
55	B8	76	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	1225	A

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Mol	Chain	Res	Type
22	BA	125	A
22	BA	764	A
22	BA	784	G
22	BA	984	A
22	BA	1286	A
22	BA	1608	A
22	BA	1970	A
22	BA	2099	U
22	BA	2146	C
22	BA	2162	G
22	BA	2188	U
22	BA	2189	U
22	BA	2251	OMG
22	BA	2518	A
22	BA	2873	A
55	B8	2	G
55	B8	3	G
55	B8	19	G
55	B8	20	U

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

40 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	6MZ	BA	1618	22	18,25,26	2.91	4 (22%)	16,36,39	1.95	3 (18%)
34	4D4	BM	81	34	9,11,12	2.52	3 (33%)	8,13,15	1.06	0
22	OMC	BA	2498	22,56	15,22,23	3.26	6 (40%)	17,31,34	1.41	3 (17%)
1	2MG	AA	1207	57,1	19,26,27	4.54	7 (36%)	21,38,41	2.36	8 (38%)
1	UR3	AA	1498	1	14,22,23	2.74	4 (28%)	15,32,35	0.77	1 (6%)
22	2MG	BA	1835	22	19,26,27	4.08	8 (42%)	21,38,41	2.30	8 (38%)
22	5MU	BA	747	22	15,22,23	1.30	2 (13%)	16,32,35	2.76	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	OMG	BA	2251	22,57,55	18,26,27	3.47	8 (44%)	20,38,41	2.24	9 (45%)
55	G7M	B8	46	55	20,26,27	3.32	7 (35%)	20,39,42	3.02	7 (35%)
1	5MC	AA	967	1	15,22,23	2.96	5 (33%)	19,32,35	1.31	2 (10%)
22	PSU	BA	1917	22	17,21,22	3.66	9 (52%)	20,30,33	3.15	6 (30%)
22	2MG	BA	2445	22	19,26,27	4.23	7 (36%)	21,38,41	2.45	8 (38%)
22	5MC	BA	1962	22,57	15,22,23	2.93	5 (33%)	19,32,35	1.17	2 (10%)
25	MEQ	BD	150	25	8,9,10	1.64	2 (25%)	5,10,12	1.76	2 (40%)
1	5MC	AA	1407	1	15,22,23	2.94	5 (33%)	19,32,35	1.35	2 (10%)
1	G7M	AA	527	1	20,26,27	3.64	6 (30%)	20,39,42	3.16	6 (30%)
22	PSU	BA	2504	22,57	17,21,22	3.63	8 (47%)	20,30,33	3.26	7 (35%)
22	PSU	BA	955	22	17,21,22	3.69	8 (47%)	20,30,33	3.43	6 (30%)
1	2MG	AA	1516	1	19,26,27	4.37	7 (36%)	21,38,41	2.24	8 (38%)
55	1MG	B8	37	55	18,26,27	3.62	7 (38%)	19,39,42	1.43	2 (10%)
22	PSU	BA	2604	22	17,21,22	3.46	8 (47%)	20,30,33	3.16	6 (30%)
22	PSU	BA	2605	22	17,21,22	3.50	8 (47%)	20,30,33	3.25	6 (30%)
22	6MZ	BA	2030	22	18,25,26	2.75	5 (27%)	16,36,39	2.70	4 (25%)
22	5MU	BA	1939	22,57	15,22,23	1.12	1 (6%)	16,32,35	2.67	1 (6%)
22	3TD	BA	1915	22	17,22,23	4.77	8 (47%)	19,32,35	1.23	3 (15%)
12	D2T	AL	89	12	4,9,10	1.11	0	3,11,13	2.71	1 (33%)
1	MA6	AA	1519	1	19,26,27	1.18	1 (5%)	18,38,41	3.59	2 (11%)
22	OMU	BA	2552	22,56	14,22,23	3.37	5 (35%)	14,31,34	0.63	0
1	PSU	AA	516	1,56	17,21,22	3.75	9 (52%)	20,30,33	3.25	6 (30%)
22	PSU	BA	2580	22,57	17,21,22	3.56	9 (52%)	20,30,33	3.18	6 (30%)
22	PSU	BA	2457	22	17,21,22	3.61	9 (52%)	20,30,33	3.15	6 (30%)
22	PSU	BA	1911	22	17,21,22	3.63	8 (47%)	20,30,33	3.04	6 (30%)
22	2MA	BA	2503	22,57,56	17,25,26	3.77	5 (29%)	19,37,40	1.86	4 (21%)
1	MA6	AA	1518	1	19,26,27	1.21	1 (5%)	18,38,41	3.51	2 (11%)
1	2MG	AA	966	1	19,26,27	4.40	7 (36%)	21,38,41	2.22	8 (38%)
22	G7M	BA	2069	22,57	20,26,27	3.48	7 (35%)	20,39,42	2.99	7 (35%)
1	4OC	AA	1402	1,56	16,23,24	3.41	6 (37%)	17,32,35	1.18	2 (11%)
22	1MG	BA	745	22	18,26,27	3.69	7 (38%)	19,39,42	1.86	4 (21%)
22	PSU	BA	746	22,56	17,21,22	3.62	9 (52%)	20,30,33	3.09	7 (35%)
55	PSU	B8	55	55	17,21,22	3.59	9 (52%)	20,30,33	2.98	7 (35%)

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	6MZ	BA	1618	22	-	0/5/27/28	0/3/3/3
34	4D4	BM	81	34	-	3/11/12/14	-
22	OMC	BA	2498	22,56	-	0/7/27/28	0/2/2/2
1	2MG	AA	1207	57,1	-	0/5/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/5/25/26	0/2/2/2
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
22	5MU	BA	747	22	-	1/5/25/26	0/2/2/2
22	OMG	BA	2251	22,57,55	-	3/5/27/28	0/3/3/3
55	G7M	B8	46	55	-	0/3/25/26	0/3/3/3
1	5MC	AA	967	1	-	0/5/25/26	0/2/2/2
22	PSU	BA	1917	22	-	0/7/25/26	0/2/2/2
22	2MG	BA	2445	22	-	1/5/27/28	0/3/3/3
22	5MC	BA	1962	22,57	-	2/5/25/26	0/2/2/2
25	MEQ	BD	150	25	-	3/8/9/11	-
1	5MC	AA	1407	1	-	0/5/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
22	PSU	BA	2504	22,57	-	2/7/25/26	0/2/2/2
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
55	1MG	B8	37	55	-	0/3/25/26	0/3/3/3
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
22	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
22	5MU	BA	1939	22,57	-	0/5/25/26	0/2/2/2
22	3TD	BA	1915	22	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/3/12/14	-
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
22	OMU	BA	2552	22,56	-	1/7/27/28	0/2/2/2
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
22	PSU	BA	2580	22,57	-	0/7/25/26	0/2/2/2
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
22	2MA	BA	2503	22,57,56	-	2/3/25/26	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
22	G7M	BA	2069	22,57	-	2/3/25/26	0/3/3/3
1	4OC	AA	1402	1,56	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
22	PSU	BA	746	22,56	-	3/7/25/26	0/2/2/2
55	PSU	B8	55	55	-	2/7/25/26	0/2/2/2

All (240) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C5-C1'	-15.10	1.39	1.52
1	AA	1207	2MG	C2-N2	13.60	1.45	1.34
1	AA	966	2MG	C2-N2	13.45	1.45	1.34
1	AA	1516	2MG	C2-N2	13.18	1.45	1.34
22	BA	2445	2MG	C2-N2	12.32	1.44	1.34
22	BA	1835	2MG	C2-N2	11.88	1.44	1.34
22	BA	1618	6MZ	C6-N6	10.99	1.53	1.35
22	BA	2030	6MZ	C6-N6	10.27	1.51	1.35
1	AA	527	G7M	C4-N3	9.21	1.50	1.35
1	AA	1207	2MG	C4-N3	8.88	1.49	1.35
22	BA	2069	G7M	C4-N3	8.86	1.49	1.35
55	B8	37	1MG	C4-N3	8.79	1.49	1.35
22	BA	745	1MG	C4-N3	8.70	1.49	1.35
1	AA	966	2MG	C4-N3	8.38	1.48	1.35
22	BA	2503	2MA	C4-N3	8.29	1.48	1.35
22	BA	2251	OMG	C4-N3	8.29	1.48	1.35
1	AA	1516	2MG	C4-N3	8.27	1.48	1.35
22	BA	2498	OMC	C6-N1	8.24	1.46	1.35
22	BA	745	1MG	C6-C5	8.15	1.54	1.41
1	AA	1402	4OC	C6-N1	8.12	1.45	1.35
1	AA	527	G7M	C6-C5	7.93	1.55	1.41
22	BA	1835	2MG	C4-N3	7.88	1.48	1.35
55	B8	46	G7M	C4-N3	7.85	1.48	1.35
22	BA	2445	2MG	C4-N3	7.85	1.48	1.35
22	BA	2445	2MG	C6-C5	7.79	1.54	1.41
22	BA	2503	2MA	C6-C5	7.77	1.53	1.41
22	BA	2069	G7M	C6-C5	7.72	1.54	1.41
55	B8	37	1MG	C2-N3	7.68	1.46	1.34
1	AA	516	PSU	C4-N3	7.68	1.46	1.33
22	BA	1917	PSU	C4-N3	7.60	1.46	1.33
55	B8	37	1MG	C6-C5	7.54	1.53	1.41
22	BA	955	PSU	C4-N3	7.53	1.46	1.33
1	AA	1207	2MG	C6-C5	7.48	1.54	1.41
22	BA	745	1MG	C2-N3	7.47	1.45	1.34
1	AA	1516	2MG	C6-C5	7.43	1.54	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1911	PSU	C4-N3	7.29	1.45	1.33
22	BA	2457	PSU	C4-N3	7.26	1.45	1.33
22	BA	2552	OMU	C4-N3	7.22	1.45	1.33
55	B8	55	PSU	C4-N3	7.21	1.45	1.33
22	BA	1915	3TD	C6-C5	7.17	1.49	1.38
22	BA	2580	PSU	C4-N3	7.15	1.45	1.33
22	BA	1835	2MG	C6-C5	7.04	1.53	1.41
22	BA	2503	2MA	C2-N3	7.03	1.46	1.34
1	AA	967	5MC	C4-N3	7.03	1.45	1.35
22	BA	2504	PSU	C4-N3	7.02	1.45	1.33
22	BA	2552	OMU	C6-N1	7.02	1.44	1.35
22	BA	746	PSU	C6-C5	7.01	1.49	1.38
22	BA	2604	PSU	C4-N3	6.94	1.45	1.33
22	BA	2504	PSU	C6-C5	6.91	1.48	1.38
1	AA	516	PSU	C6-C5	6.91	1.48	1.38
55	B8	46	G7M	C6-C5	6.90	1.53	1.41
1	AA	527	G7M	C6-N1	6.90	1.45	1.33
1	AA	966	2MG	C6-C5	6.84	1.53	1.41
22	BA	2580	PSU	C6-C5	6.79	1.48	1.38
22	BA	2605	PSU	C4-N3	6.72	1.44	1.33
1	AA	1407	5MC	C4-N3	6.70	1.44	1.35
55	B8	46	G7M	C6-N1	6.70	1.44	1.33
22	BA	2251	OMG	C6-C5	6.69	1.52	1.41
22	BA	1911	PSU	C6-C5	6.69	1.48	1.38
22	BA	746	PSU	C4-N3	6.65	1.44	1.33
22	BA	2069	G7M	C6-N1	6.65	1.44	1.33
22	BA	2605	PSU	C6-C5	6.63	1.48	1.38
22	BA	955	PSU	C6-C5	6.59	1.48	1.38
22	BA	2457	PSU	C6-C5	6.57	1.48	1.38
22	BA	1917	PSU	C6-C5	6.56	1.48	1.38
22	BA	1962	5MC	C4-N3	6.54	1.44	1.35
22	BA	2604	PSU	C6-C5	6.52	1.48	1.38
55	B8	55	PSU	C6-C5	6.49	1.48	1.38
1	AA	1498	UR3	C6-N1	6.44	1.43	1.35
22	BA	2503	2MA	C2-N1	6.11	1.44	1.34
1	AA	1207	2MG	C6-N1	6.10	1.43	1.33
34	BM	81	4D4	CZ-NE	6.09	1.45	1.33
55	B8	55	PSU	C2-N1	5.99	1.50	1.38
1	AA	516	PSU	C2-N3	5.99	1.50	1.38
1	AA	966	2MG	C6-N1	5.96	1.43	1.33
22	BA	1911	PSU	C2-N1	5.95	1.50	1.38
22	BA	2580	PSU	C2-N3	5.91	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	516	PSU	C2-N1	5.84	1.49	1.38
22	BA	746	PSU	C2-N1	5.79	1.49	1.38
22	BA	1911	PSU	C2-N3	5.77	1.49	1.38
22	BA	2445	2MG	C6-N1	5.76	1.43	1.33
22	BA	1917	PSU	C2-N1	5.72	1.49	1.38
22	BA	1917	PSU	C2-N3	5.71	1.49	1.38
22	BA	2605	PSU	C2-N1	5.68	1.49	1.38
1	AA	1516	2MG	C6-N1	5.67	1.42	1.33
22	BA	2504	PSU	C2-N1	5.66	1.49	1.38
22	BA	955	PSU	C2-N3	5.65	1.49	1.38
55	B8	55	PSU	C2-N3	5.62	1.49	1.38
22	BA	2552	OMU	C2-N3	5.60	1.49	1.38
22	BA	2251	OMG	C2-N2	5.57	1.45	1.33
22	BA	2504	PSU	C2-N3	5.56	1.49	1.38
22	BA	2457	PSU	C2-N3	5.55	1.49	1.38
22	BA	2604	PSU	C2-N3	5.54	1.49	1.38
22	BA	1962	5MC	C5-C4	5.51	1.49	1.41
22	BA	2604	PSU	C2-N1	5.51	1.49	1.38
22	BA	1835	2MG	C6-N1	5.43	1.42	1.33
1	AA	1402	4OC	C6-C5	5.43	1.50	1.38
22	BA	746	PSU	C2-N3	5.38	1.48	1.38
1	AA	527	G7M	C2-N1	5.29	1.44	1.35
22	BA	955	PSU	C2-N1	5.29	1.48	1.38
22	BA	2251	OMG	C6-N1	5.29	1.42	1.33
22	BA	2580	PSU	C2-N1	5.28	1.48	1.38
1	AA	967	5MC	C2-N3	5.27	1.48	1.38
22	BA	2457	PSU	C2-N1	5.26	1.48	1.38
22	BA	955	PSU	C5-C1'	5.23	1.56	1.52
22	BA	1915	3TD	C2-N1	5.21	1.48	1.38
1	AA	1402	4OC	C2-N3	5.21	1.48	1.38
22	BA	1915	3TD	C4-N3	5.17	1.45	1.38
55	B8	46	G7M	C2-N1	5.17	1.44	1.35
1	AA	1407	5MC	C2-N3	5.10	1.48	1.38
22	BA	1915	3TD	C6-N1	5.08	1.45	1.34
1	AA	1402	4OC	C4-N3	5.05	1.44	1.34
22	BA	2457	PSU	C5-C1'	5.01	1.56	1.52
1	AA	527	G7M	C2-N2	4.99	1.43	1.33
1	AA	1407	5MC	C5-C4	4.96	1.49	1.41
22	BA	1962	5MC	C2-N3	4.95	1.48	1.38
22	BA	2605	PSU	C2-N3	4.93	1.47	1.38
22	BA	2498	OMC	C2-N3	4.90	1.47	1.38
22	BA	2251	OMG	C2-N1	4.90	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2498	OMC	C6-C5	4.89	1.48	1.38
22	BA	1917	PSU	C6-N1	4.80	1.44	1.34
55	B8	55	PSU	C6-N1	4.75	1.44	1.34
22	BA	2069	G7M	C2-N1	4.73	1.43	1.35
22	BA	2498	OMC	C4-N3	4.71	1.43	1.35
22	BA	1911	PSU	C6-N1	4.70	1.44	1.34
22	BA	746	PSU	C5-C1'	4.70	1.56	1.52
1	AA	967	5MC	C5-C4	4.70	1.48	1.41
22	BA	2069	G7M	C2-N2	4.67	1.43	1.33
22	BA	2605	PSU	C6-N1	4.66	1.44	1.34
1	AA	516	PSU	C6-N1	4.66	1.44	1.34
22	BA	2504	PSU	C6-N1	4.55	1.44	1.34
1	AA	1498	UR3	C6-C5	4.50	1.48	1.38
22	BA	955	PSU	C6-N1	4.44	1.43	1.34
22	BA	746	PSU	C6-N1	4.43	1.43	1.34
22	BA	2457	PSU	C6-N1	4.43	1.43	1.34
1	AA	1498	UR3	C4-N3	4.43	1.44	1.38
55	B8	46	G7M	C2-N2	4.34	1.42	1.33
1	AA	1407	5MC	C4-N4	4.33	1.45	1.34
1	AA	967	5MC	C4-N4	4.33	1.45	1.34
22	BA	2605	PSU	C5-C1'	4.33	1.55	1.52
1	AA	1402	4OC	C4-N4	4.30	1.45	1.36
55	B8	37	1MG	C2-N2	4.29	1.42	1.33
22	BA	2504	PSU	C5-C1'	4.29	1.55	1.52
22	BA	2604	PSU	C6-N1	4.28	1.43	1.34
22	BA	2580	PSU	C6-N1	4.25	1.43	1.34
22	BA	2503	2MA	C6-N1	4.21	1.43	1.35
22	BA	745	1MG	C2-N2	4.20	1.42	1.33
1	AA	516	PSU	C5-C1'	4.19	1.55	1.52
1	AA	1402	4OC	C5-C4	4.15	1.49	1.39
22	BA	2552	OMU	C6-C5	4.13	1.47	1.38
1	AA	1498	UR3	O4-C4	-4.12	1.14	1.24
22	BA	1917	PSU	C5-C1'	4.10	1.55	1.52
22	BA	1962	5MC	C4-N4	4.10	1.44	1.34
22	BA	1915	3TD	C4-C5	4.04	1.50	1.41
22	BA	2504	PSU	C4-C5	3.89	1.49	1.41
1	AA	1207	2MG	C2-N3	3.80	1.46	1.34
22	BA	2604	PSU	C4-C5	3.71	1.49	1.41
22	BA	1911	PSU	C5-C1'	3.65	1.55	1.52
22	BA	2580	PSU	C5-C1'	3.61	1.55	1.52
1	AA	966	2MG	C2-N3	3.58	1.45	1.34
1	AA	1516	2MG	C2-N3	3.56	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	955	PSU	C4-C5	3.56	1.49	1.41
22	BA	2605	PSU	C4-C5	3.54	1.49	1.41
1	AA	1407	5MC	C6-C5	3.52	1.49	1.40
22	BA	747	5MU	C4-N3	3.50	1.39	1.33
22	BA	745	1MG	C6-N1	3.49	1.43	1.38
22	BA	1917	PSU	C4-C5	3.47	1.48	1.41
22	BA	1911	PSU	C4-C5	3.46	1.48	1.41
55	B8	55	PSU	C5-C1'	3.43	1.55	1.52
22	BA	746	PSU	C4-C5	3.40	1.48	1.41
1	AA	516	PSU	C4-C5	3.37	1.48	1.41
22	BA	1835	2MG	C2-N3	3.33	1.44	1.34
22	BA	2457	PSU	C4-C5	3.30	1.48	1.41
22	BA	2445	2MG	C2-N3	3.30	1.44	1.34
1	AA	967	5MC	C6-C5	3.29	1.49	1.40
22	BA	1962	5MC	C6-C5	3.27	1.49	1.40
1	AA	1207	2MG	C2-N1	3.23	1.44	1.34
22	BA	1618	6MZ	C2-N3	3.21	1.37	1.32
1	AA	966	2MG	C2-N1	3.19	1.44	1.34
1	AA	1516	2MG	C2-N1	3.17	1.44	1.34
55	B8	55	PSU	C4-C5	3.13	1.48	1.41
22	BA	2580	PSU	C4-C5	3.13	1.48	1.41
22	BA	2498	OMC	C4-N4	3.11	1.44	1.35
22	BA	745	1MG	O6-C6	-3.10	1.16	1.24
34	BM	81	4D4	CZ-NH2	3.04	1.44	1.32
22	BA	1835	2MG	C2-N1	3.04	1.43	1.34
25	BD	150	MEQ	OE1-CD	-3.03	1.17	1.23
22	BA	2604	PSU	C5-C1'	2.97	1.54	1.52
55	B8	37	1MG	C6-N1	2.97	1.42	1.38
22	BA	2498	OMC	C5-C4	2.94	1.48	1.41
22	BA	2445	2MG	C2-N1	2.94	1.43	1.34
1	AA	1518	MA6	C5-C4	-2.88	1.33	1.40
22	BA	2030	6MZ	C2-N3	2.82	1.36	1.32
22	BA	1835	2MG	O6-C6	-2.76	1.17	1.24
22	BA	1939	5MU	C4-N3	2.75	1.37	1.33
1	AA	527	G7M	C2-N3	2.74	1.47	1.34
55	B8	46	G7M	C5-C4	-2.73	1.35	1.39
22	BA	2552	OMU	O4-C4	-2.70	1.17	1.24
22	BA	2445	2MG	O6-C6	-2.70	1.17	1.24
22	BA	2251	OMG	O6-C6	-2.68	1.17	1.24
1	AA	1519	MA6	C5-C4	-2.67	1.33	1.40
22	BA	2030	6MZ	C5-C4	-2.59	1.34	1.40
55	B8	37	1MG	O6-C6	-2.57	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	B8	55	PSU	O4'-C1'	-2.56	1.40	1.44
22	BA	2580	PSU	O4'-C1'	-2.52	1.40	1.44
22	BA	1618	6MZ	C9-N6	2.49	1.49	1.45
22	BA	955	PSU	O4-C4	-2.48	1.18	1.24
22	BA	2457	PSU	O4-C4	-2.47	1.18	1.24
22	BA	747	5MU	C4-C5	2.47	1.46	1.41
22	BA	2604	PSU	O4-C4	-2.46	1.18	1.24
22	BA	1618	6MZ	C5-C4	-2.46	1.34	1.40
1	AA	1516	2MG	O6-C6	-2.41	1.18	1.24
22	BA	2069	G7M	C2-N3	2.39	1.45	1.34
22	BA	746	PSU	O4'-C1'	-2.38	1.41	1.44
34	BM	81	4D4	CZ-NH1	-2.36	1.25	1.34
1	AA	516	PSU	O4'-C1'	-2.35	1.41	1.44
1	AA	966	2MG	O6-C6	-2.35	1.18	1.24
55	B8	46	G7M	C2-N3	2.35	1.45	1.34
55	B8	55	PSU	O4-C4	-2.30	1.18	1.24
22	BA	2580	PSU	O4-C4	-2.29	1.18	1.24
22	BA	1915	3TD	O4-C4	-2.29	1.18	1.24
1	AA	1207	2MG	O6-C6	-2.27	1.18	1.24
22	BA	746	PSU	O4-C4	-2.23	1.19	1.24
22	BA	2251	OMG	C2-N3	2.22	1.45	1.34
22	BA	2605	PSU	O4-C4	-2.20	1.19	1.24
25	BD	150	MEQ	CD-NE2	2.19	1.44	1.34
22	BA	2030	6MZ	C9-N6	2.19	1.48	1.45
22	BA	2504	PSU	O4-C4	-2.18	1.19	1.24
22	BA	2251	OMG	C5-C4	-2.17	1.35	1.40
55	B8	37	1MG	C5-C4	-2.13	1.35	1.40
22	BA	745	1MG	C5-C4	-2.12	1.35	1.40
22	BA	1915	3TD	O4'-C1'	-2.11	1.41	1.44
22	BA	1917	PSU	O4'-C1'	-2.08	1.41	1.44
22	BA	2457	PSU	O4'-C1'	-2.07	1.41	1.44
1	AA	516	PSU	O4-C4	-2.06	1.19	1.24
22	BA	2030	6MZ	C5-N7	-2.06	1.32	1.39
22	BA	1835	2MG	C5-C4	-2.04	1.35	1.40
22	BA	1911	PSU	O4-C4	-2.02	1.19	1.24
22	BA	1917	PSU	O4-C4	-2.01	1.19	1.24
22	BA	2069	G7M	C5-C4	-2.00	1.36	1.39

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1519	MA6	N1-C6-N6	-13.93	102.40	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1518	MA6	N1-C6-N6	-13.60	102.74	117.06
22	BA	955	PSU	N1-C2-N3	-12.16	118.76	128.43
1	AA	527	G7M	C1'-N9-C4	11.40	146.68	126.64
1	AA	516	PSU	N1-C2-N3	-11.37	119.39	128.43
22	BA	2457	PSU	N1-C2-N3	-11.24	119.50	128.43
22	BA	1917	PSU	N1-C2-N3	-11.12	119.59	128.43
22	BA	2605	PSU	N1-C2-N3	-10.86	119.80	128.43
22	BA	747	5MU	C4-N3-C2	10.73	124.20	115.14
55	B8	46	G7M	C1'-N9-C4	10.63	145.31	126.64
22	BA	2580	PSU	N1-C2-N3	-10.52	120.07	128.43
55	B8	55	PSU	N1-C2-N3	-10.51	120.08	128.43
22	BA	1911	PSU	N1-C2-N3	-10.49	120.09	128.43
22	BA	2604	PSU	N1-C2-N3	-10.35	120.20	128.43
22	BA	2504	PSU	N1-C2-N3	-10.34	120.21	128.43
22	BA	1939	5MU	C4-N3-C2	10.27	123.81	115.14
22	BA	746	PSU	N1-C2-N3	-10.14	120.36	128.43
22	BA	2069	G7M	C1'-N9-C4	9.20	142.80	126.64
22	BA	2030	6MZ	C9-N6-C6	-7.09	116.76	122.87
1	AA	516	PSU	C4-N3-C2	6.29	120.45	115.14
22	BA	955	PSU	C4-N3-C2	6.14	120.32	115.14
22	BA	2069	G7M	N3-C2-N1	-6.09	119.10	127.22
22	BA	2503	2MA	C2-N3-C4	6.00	120.39	115.52
22	BA	2605	PSU	C4-N3-C2	5.93	120.15	115.14
22	BA	745	1MG	C2-N3-C4	5.70	121.87	115.36
22	BA	1917	PSU	C4-N3-C2	5.70	119.95	115.14
22	BA	2580	PSU	C4-N3-C2	5.66	119.92	115.14
22	BA	2504	PSU	C4-N3-C2	5.57	119.84	115.14
1	AA	1518	MA6	N3-C2-N1	-5.56	119.99	128.68
22	BA	1618	6MZ	N3-C2-N1	-5.55	120.00	128.68
22	BA	2030	6MZ	N3-C2-N1	-5.55	120.00	128.68
22	BA	2251	OMG	N3-C2-N1	-5.50	119.89	127.22
1	AA	1519	MA6	N3-C2-N1	-5.45	120.16	128.68
22	BA	2445	2MG	C2-N3-C4	5.40	121.40	115.28
22	BA	746	PSU	C4-N3-C2	5.36	119.67	115.14
1	AA	527	G7M	N3-C2-N1	-5.31	120.14	127.22
22	BA	2457	PSU	C4-N3-C2	5.31	119.62	115.14
22	BA	2504	PSU	C5-C1'-C2'	-5.26	105.93	115.32
22	BA	2604	PSU	C4-N3-C2	5.16	119.50	115.14
22	BA	1911	PSU	C4-N3-C2	5.15	119.49	115.14
22	BA	2445	2MG	N2-C2-N1	4.99	121.75	116.96
22	BA	2580	PSU	C5-C4-N3	-4.78	119.20	125.36
55	B8	46	G7M	N3-C2-N1	-4.77	120.86	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1207	2MG	C2-N3-C4	4.74	120.65	115.28
1	AA	966	2MG	C1'-N9-C4	4.65	134.81	126.64
22	BA	1835	2MG	N2-C2-N1	4.64	121.42	116.96
1	AA	1207	2MG	C1'-N9-C4	4.64	134.79	126.64
22	BA	2069	G7M	C2-N3-C4	4.49	120.49	115.36
1	AA	516	PSU	C5-C4-N3	-4.46	119.61	125.36
22	BA	1835	2MG	CM2-N2-C2	-4.46	118.21	123.59
22	BA	1835	2MG	C1'-N9-C4	4.46	134.47	126.64
12	AL	89	D2T	CB1-SB-CB	4.36	110.43	101.85
55	B8	55	PSU	C4-N3-C2	4.34	118.81	115.14
22	BA	2030	6MZ	C2-N1-C6	4.33	120.30	116.59
22	BA	2604	PSU	C5-C4-N3	-4.30	119.82	125.36
22	BA	2445	2MG	N3-C2-N1	-4.28	119.47	126.23
1	AA	1516	2MG	N2-C2-N1	4.27	121.06	116.96
1	AA	1207	2MG	N2-C2-N1	4.27	121.06	116.96
22	BA	2504	PSU	C5-C4-N3	-4.26	119.87	125.36
22	BA	2604	PSU	C5-C1'-C2'	-4.26	107.72	115.32
22	BA	1917	PSU	C5-C4-N3	-4.14	120.03	125.36
1	AA	1516	2MG	C2-N3-C4	4.11	119.94	115.28
22	BA	2498	OMC	C2-N3-C4	4.11	120.50	116.34
55	B8	37	1MG	C1'-N9-C4	-4.10	119.44	126.64
1	AA	1207	2MG	N3-C2-N1	-4.10	119.75	126.23
1	AA	966	2MG	C2-N3-C4	4.06	119.89	115.28
22	BA	1911	PSU	C5-C4-N3	-4.06	120.13	125.36
22	BA	746	PSU	C5-C4-N3	-4.04	120.15	125.36
22	BA	2445	2MG	C1'-N9-C4	4.02	133.71	126.64
22	BA	1618	6MZ	C2-N1-C6	4.00	120.02	116.59
1	AA	966	2MG	N2-C2-N1	4.00	120.80	116.96
22	BA	2605	PSU	C5-C4-N3	-4.00	120.21	125.36
22	BA	1835	2MG	C2-N3-C4	3.99	119.81	115.28
1	AA	527	G7M	C2-N3-C4	3.98	119.91	115.36
1	AA	1407	5MC	C2-N3-C4	3.98	120.83	116.02
1	AA	966	2MG	N3-C2-N1	-3.97	119.95	126.23
22	BA	745	1MG	C1'-N9-C4	-3.90	119.78	126.64
22	BA	1962	5MC	C2-N3-C4	3.89	120.72	116.02
22	BA	955	PSU	C5-C4-N3	-3.85	120.40	125.36
1	AA	1516	2MG	CM2-N2-C2	-3.85	118.94	123.59
1	AA	1516	2MG	N3-C2-N1	-3.78	120.25	126.23
55	B8	37	1MG	C2-N3-C4	3.75	119.64	115.36
22	BA	2457	PSU	C5-C4-N3	-3.75	120.53	125.36
55	B8	55	PSU	C5-C6-N1	-3.74	119.84	124.44
55	B8	46	G7M	N2-C2-N1	3.71	123.02	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	967	5MC	C2-N3-C4	3.70	120.48	116.02
1	AA	1516	2MG	C1'-N9-C4	3.67	133.09	126.64
22	BA	2251	OMG	C2-N3-C4	3.58	119.45	115.36
22	BA	1835	2MG	N3-C2-N1	-3.50	120.70	126.23
55	B8	55	PSU	C5-C4-N3	-3.46	120.90	125.36
22	BA	2604	PSU	C5-C6-N1	-3.40	120.26	124.44
1	AA	1207	2MG	CM2-N2-C2	-3.39	119.50	123.59
22	BA	2605	PSU	C5-C1'-C2'	-3.34	109.36	115.32
22	BA	746	PSU	C5-C1'-C2'	-3.34	109.37	115.32
22	BA	955	PSU	C5-C1'-C2'	-3.33	109.39	115.32
22	BA	2251	OMG	O3'-C3'-C2'	3.32	120.59	111.17
22	BA	746	PSU	O4'-C1'-C5	3.32	115.07	109.93
22	BA	2605	PSU	C5-C6-N1	-3.25	120.44	124.44
22	BA	2503	2MA	N3-C2-N1	-3.21	119.81	125.72
22	BA	2030	6MZ	C1'-N9-C4	-3.21	121.00	126.64
22	BA	746	PSU	C5-C6-N1	-3.20	120.51	124.44
22	BA	2580	PSU	C5-C6-N1	-3.19	120.52	124.44
22	BA	955	PSU	C6-N1-C2	3.15	120.55	115.36
22	BA	1911	PSU	C5-C6-N1	-3.14	120.58	124.44
22	BA	2445	2MG	CM2-N2-C2	-3.13	119.82	123.59
22	BA	1915	3TD	C5-C6-N1	-3.10	120.63	124.44
22	BA	2457	PSU	C6-N1-C2	3.06	120.41	115.36
1	AA	1402	4OC	CM4-N4-C4	-3.06	120.34	122.97
22	BA	2504	PSU	C5-C6-N1	-3.01	120.74	124.44
22	BA	2457	PSU	C5-C6-N1	-2.98	120.77	124.44
25	BD	150	MEQ	CG-CD-NE2	2.98	120.42	116.29
22	BA	2503	2MA	C5-C6-N1	-2.96	119.96	123.06
55	B8	55	PSU	C6-N1-C2	2.92	120.18	115.36
22	BA	2069	G7M	C6-N1-C2	2.92	120.57	115.93
22	BA	2069	G7M	N2-C2-N1	2.89	121.75	117.25
22	BA	2604	PSU	C6-N1-C2	2.86	120.08	115.36
1	AA	966	2MG	CM2-N2-C2	-2.85	120.15	123.59
22	BA	2069	G7M	C6-C5-C4	-2.81	118.11	120.80
22	BA	1917	PSU	C5-C6-N1	-2.78	121.02	124.44
22	BA	2605	PSU	C6-N1-C2	2.77	119.94	115.36
55	B8	46	G7M	C5-C6-N1	-2.76	119.66	123.43
22	BA	1917	PSU	C6-N1-C2	2.72	119.85	115.36
22	BA	1915	3TD	C6-N1-C2	2.69	119.79	115.36
1	AA	527	G7M	C5-C6-N1	-2.68	119.76	123.43
22	BA	2251	OMG	N2-C2-N1	2.68	121.42	117.25
22	BA	2251	OMG	C5-C6-N1	-2.65	119.80	123.43
22	BA	2445	2MG	C4-C5-N7	-2.63	106.65	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	2580	PSU	C6-N1-C2	2.63	119.70	115.36
22	BA	2504	PSU	C6-N1-C2	2.62	119.69	115.36
22	BA	1835	2MG	C5-C6-N1	-2.62	119.85	123.43
1	AA	1516	2MG	C5-C6-N1	-2.61	119.86	123.43
22	BA	2251	OMG	C6-N1-C2	2.61	120.08	115.93
22	BA	1911	PSU	C6-N1-C2	2.61	119.66	115.36
22	BA	2580	PSU	O4'-C1'-C2'	2.56	108.81	104.66
1	AA	966	2MG	C5-C6-N1	-2.56	119.93	123.43
22	BA	2445	2MG	C6-N1-C2	2.54	119.73	115.18
1	AA	1402	4OC	C5-C4-N3	-2.53	118.89	123.16
22	BA	745	1MG	C5-C6-N1	2.53	120.90	118.20
22	BA	2251	OMG	C1'-N9-C4	2.52	131.07	126.64
1	AA	966	2MG	C6-N1-C2	2.52	119.70	115.18
1	AA	1207	2MG	C6-N1-C2	2.51	119.68	115.18
1	AA	1516	2MG	C6-N1-C2	2.50	119.66	115.18
22	BA	746	PSU	C6-N1-C2	2.48	119.46	115.36
1	AA	516	PSU	C6-N1-C2	2.47	119.43	115.36
1	AA	1207	2MG	C5-C6-N1	-2.46	120.06	123.43
1	AA	527	G7M	C6-N1-C2	2.46	119.84	115.93
55	B8	46	G7M	C2-N3-C4	2.45	118.16	115.36
22	BA	2445	2MG	C5-C6-N1	-2.45	120.08	123.43
22	BA	2069	G7M	C5-C6-N1	-2.45	120.09	123.43
22	BA	1911	PSU	C5-C1'-C2'	-2.43	110.98	115.32
55	B8	46	G7M	C6-C5-C4	-2.42	118.49	120.80
1	AA	966	2MG	N2-C2-N3	2.38	119.25	116.96
22	BA	955	PSU	C5-C6-N1	-2.36	121.54	124.44
1	AA	1207	2MG	N2-C2-N3	2.32	119.19	116.96
25	BD	150	MEQ	OE1-CD-CG	-2.31	117.79	122.02
1	AA	1516	2MG	C4-C5-N7	-2.28	107.02	109.40
1	AA	516	PSU	C5-C6-N1	-2.28	121.63	124.44
1	AA	967	5MC	N4-C4-N3	2.27	120.25	117.03
1	AA	527	G7M	N2-C2-N1	2.26	120.77	117.25
22	BA	2251	OMG	C3'-C2'-C1'	-2.26	98.65	102.89
22	BA	2498	OMC	C6-N1-C2	-2.25	117.62	121.20
22	BA	2251	OMG	O3'-C3'-C4'	2.25	117.55	111.05
55	B8	46	G7M	C6-N1-C2	2.23	119.47	115.93
22	BA	1835	2MG	C6-N1-C2	2.23	119.17	115.18
22	BA	1835	2MG	C4-C5-N7	-2.23	107.08	109.40
22	BA	745	1MG	N2-C2-N1	2.18	121.21	118.47
1	AA	1407	5MC	N4-C4-N3	2.17	120.10	117.03
22	BA	2503	2MA	CM2-C2-N1	2.15	120.51	117.15
55	B8	55	PSU	C5-C1'-C2'	-2.14	111.50	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1618	6MZ	C9-N6-C6	-2.13	121.04	122.87
22	BA	2498	OMC	C5-C4-N3	-2.12	119.27	121.72
22	BA	1962	5MC	C5-C6-N1	-2.10	119.93	122.19
1	AA	516	PSU	O4'-C1'-C2'	2.10	108.06	104.66
55	B8	55	PSU	O4'-C1'-C2'	2.10	108.06	104.66
22	BA	2457	PSU	O4'-C1'-C2'	2.09	108.05	104.66
22	BA	1917	PSU	O4'-C1'-C2'	2.07	108.01	104.66
22	BA	2504	PSU	O4'-C1'-C5	2.06	113.11	109.93
22	BA	1915	3TD	O4'-C1'-C2'	2.05	107.98	104.66
1	AA	1498	UR3	C3U-N3-C4	2.05	120.83	118.12

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
25	BD	150	MEQ	N-CA-CB-CG
25	BD	150	MEQ	C-CA-CB-CG
25	BD	150	MEQ	O-C-CA-CB
55	B8	55	PSU	O4'-C1'-C5-C4
55	B8	55	PSU	O4'-C1'-C5-C6
22	BA	1962	5MC	O4'-C1'-N1-C6
22	BA	1962	5MC	C2'-C1'-N1-C6
22	BA	2030	6MZ	O4'-C4'-C5'-O5'
22	BA	2251	OMG	C1'-C2'-O2'-CM2
1	AA	527	G7M	O4'-C4'-C5'-O5'
22	BA	2030	6MZ	C3'-C4'-C5'-O5'
22	BA	2504	PSU	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
22	BA	2504	PSU	C3'-C4'-C5'-O5'
1	AA	1402	4OC	O4'-C4'-C5'-O5'
22	BA	2251	OMG	O4'-C4'-C5'-O5'
34	BM	81	4D4	OB-CB-CG-CD
22	BA	2251	OMG	C3'-C4'-C5'-O5'
1	AA	1402	4OC	C3'-C4'-C5'-O5'
22	BA	2445	2MG	C3'-C4'-C5'-O5'
22	BA	746	PSU	C2'-C1'-C5-C6
22	BA	747	5MU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
22	BA	2069	G7M	C4'-C5'-O5'-P
22	BA	2552	OMU	C3'-C2'-O2'-CM2
22	BA	2069	G7M	O4'-C4'-C5'-O5'
22	BA	746	PSU	O4'-C1'-C5-C6
34	BM	81	4D4	CG-CD-NE-CZ
22	BA	746	PSU	O4'-C1'-C5-C4
34	BM	81	4D4	CA-CB-CG-CD
22	BA	2503	2MA	O4'-C4'-C5'-O5'
22	BA	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	BA	2251	OMG	1	0
55	B8	46	G7M	3	0
25	BD	150	MEQ	1	0
22	BA	2504	PSU	1	0
55	B8	37	1MG	2	0
22	BA	2030	6MZ	2	0
22	BA	1915	3TD	1	0
22	BA	2552	OMU	1	0
22	BA	2503	2MA	1	0
22	BA	746	PSU	1	0
55	B8	55	PSU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 477 ligands modelled in this entry, 476 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	TRP	BA	3001	-	12,16,16	0.91	0	12,22,22	1.05	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
59	TRP	BA	3001	-	-	0/3/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.28

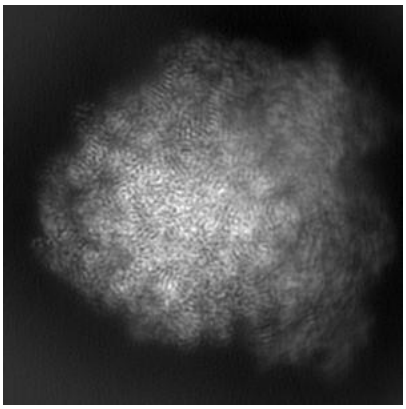
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12694. These allow visual inspection of the internal detail of the map and identification of artifacts.

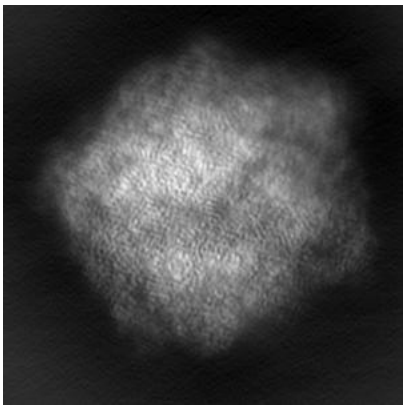
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

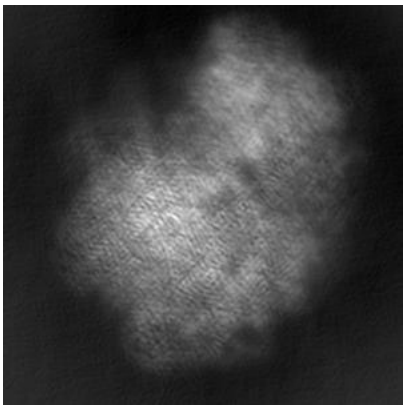
6.1.1 Primary map



X

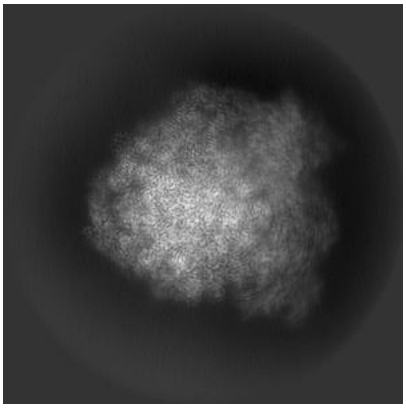


Y

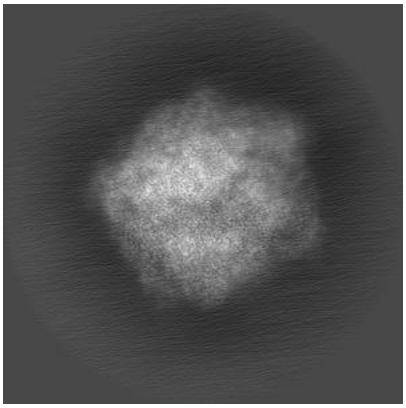


Z

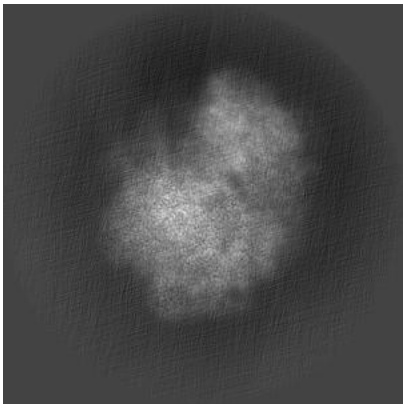
6.1.2 Raw map



X



Y

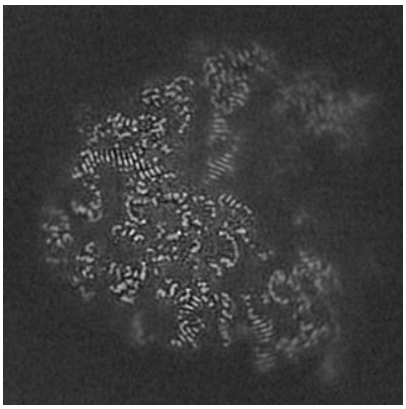


Z

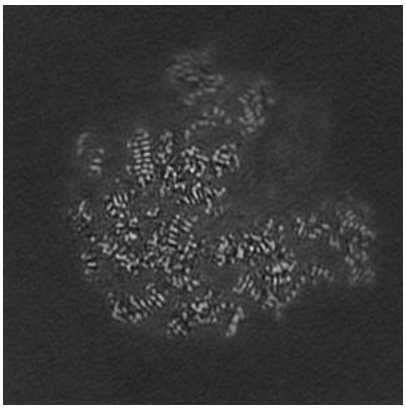
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

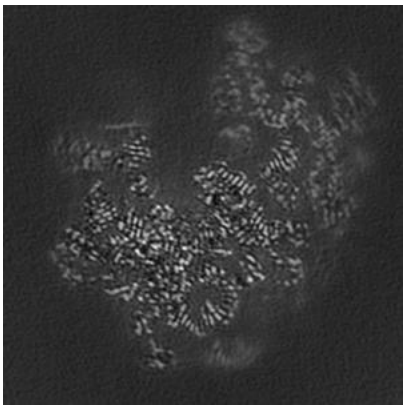
6.2.1 Primary map



X Index: 162

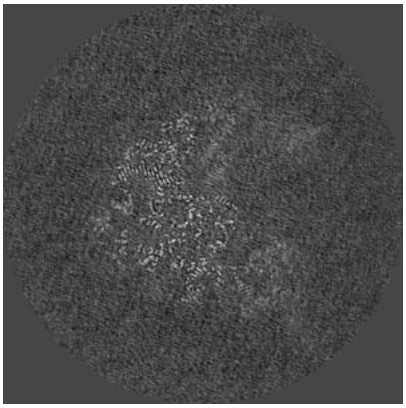


Y Index: 162

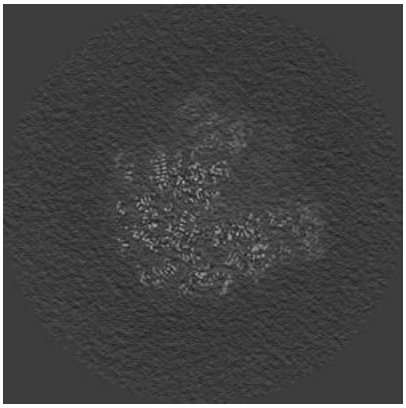


Z Index: 162

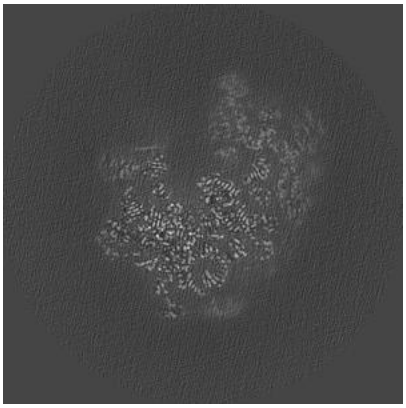
6.2.2 Raw map



X Index: 232



Y Index: 232

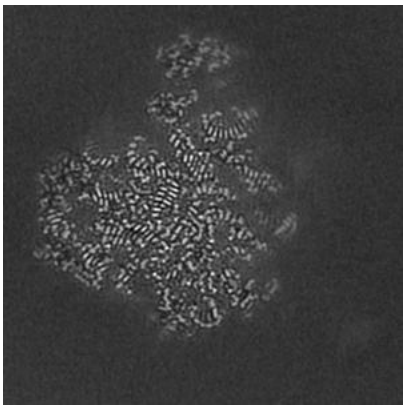


Z Index: 232

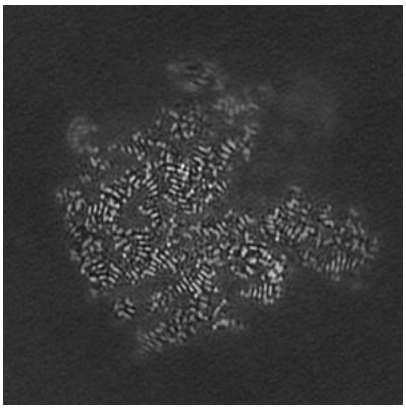
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

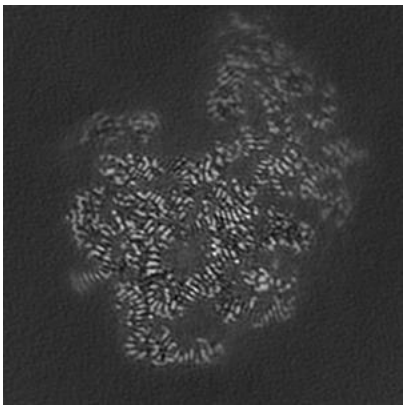
6.3.1 Primary map



X Index: 121

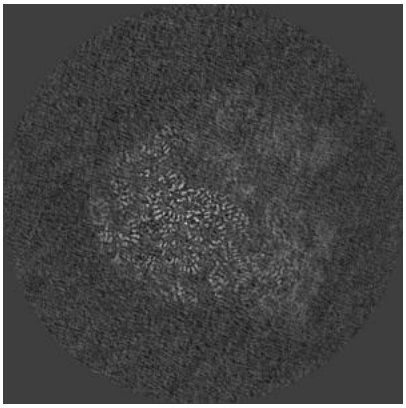


Y Index: 150

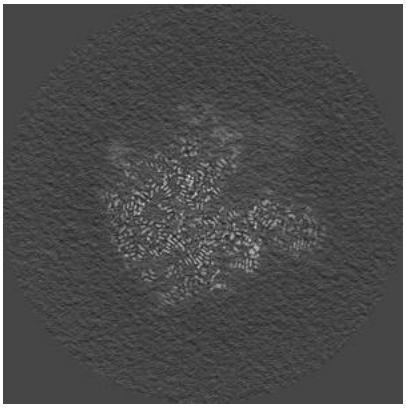


Z Index: 143

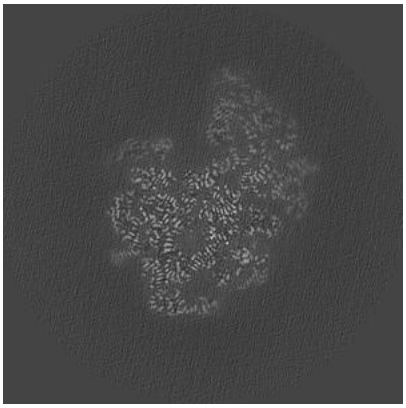
6.3.2 Raw map



X Index: 244



Y Index: 220



Z Index: 213

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

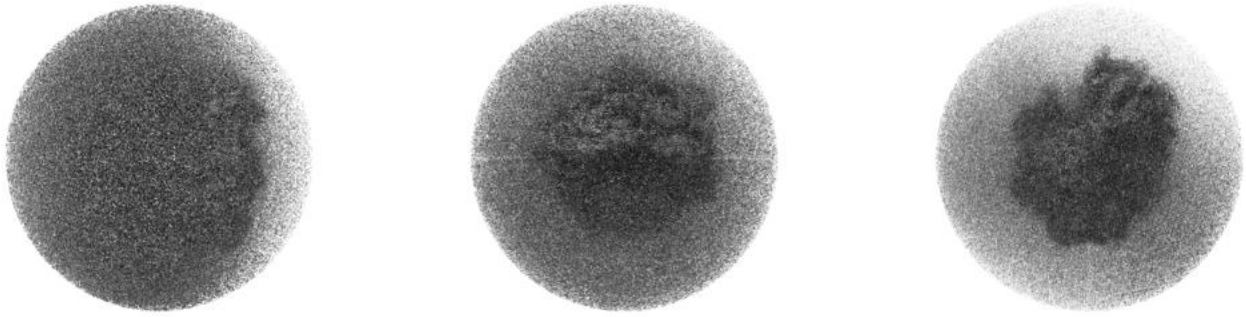
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

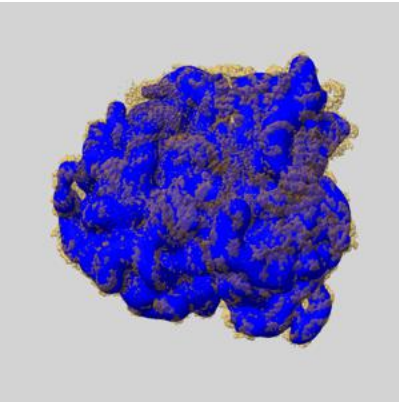
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

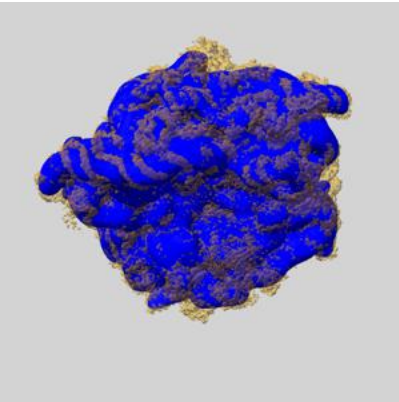
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

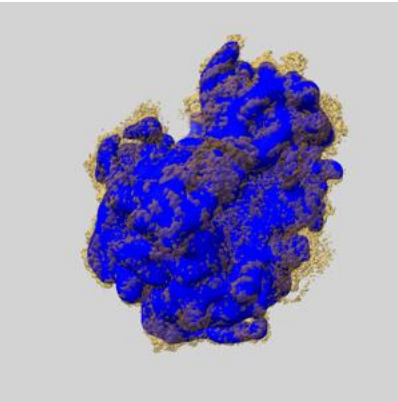
6.5.1 emd_12694_msk_1.map



X



Y

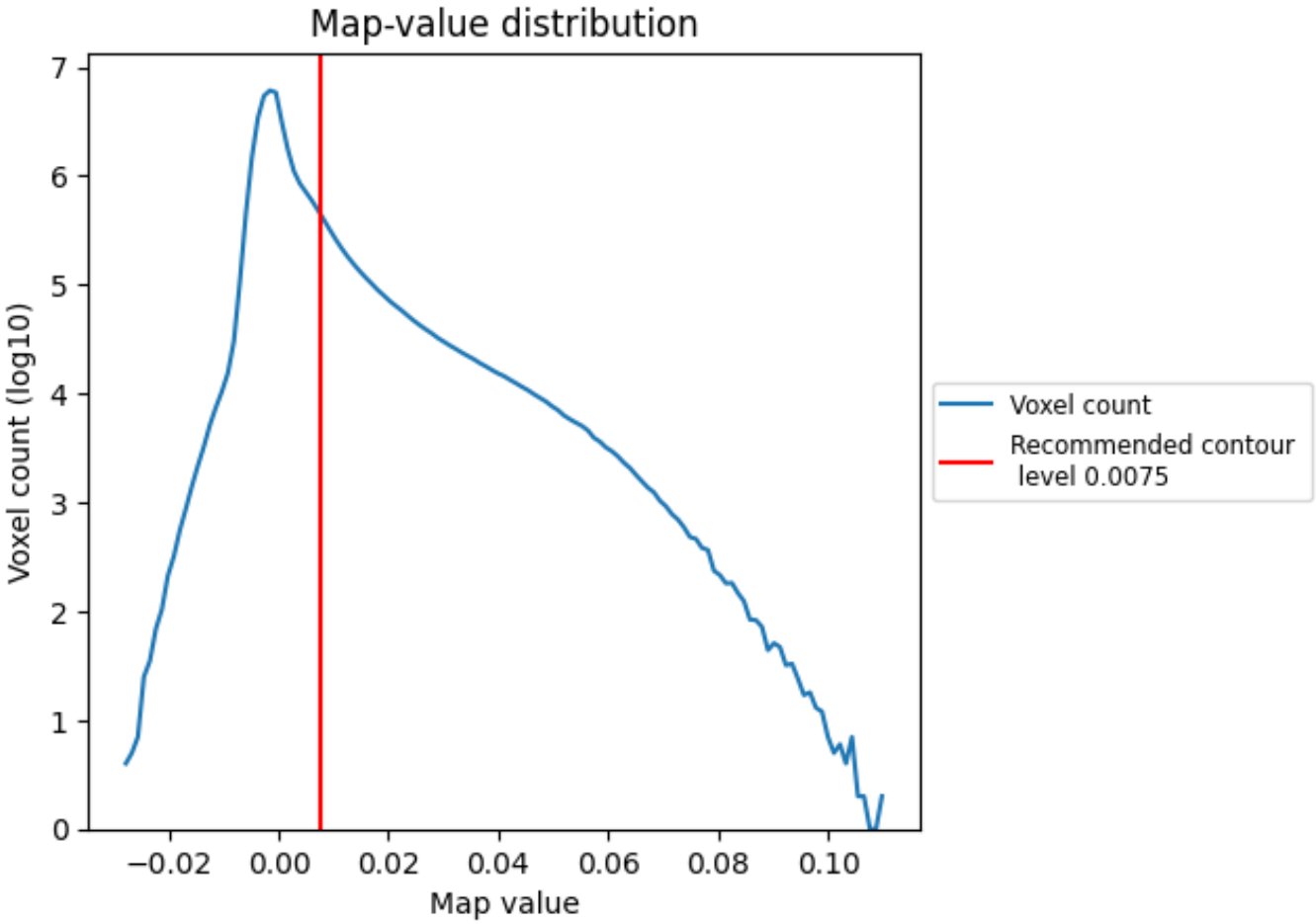


Z

7 Map analysis

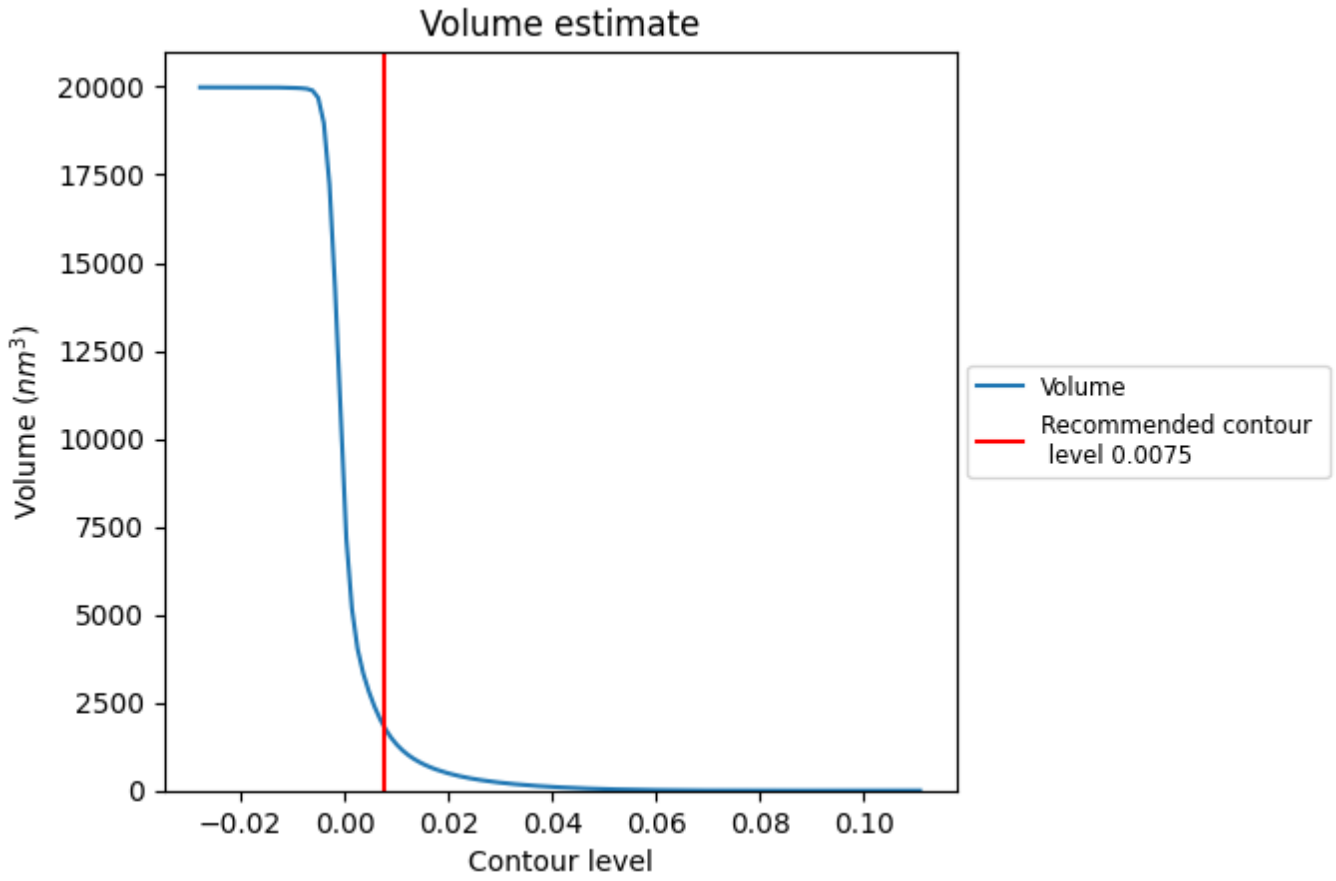
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

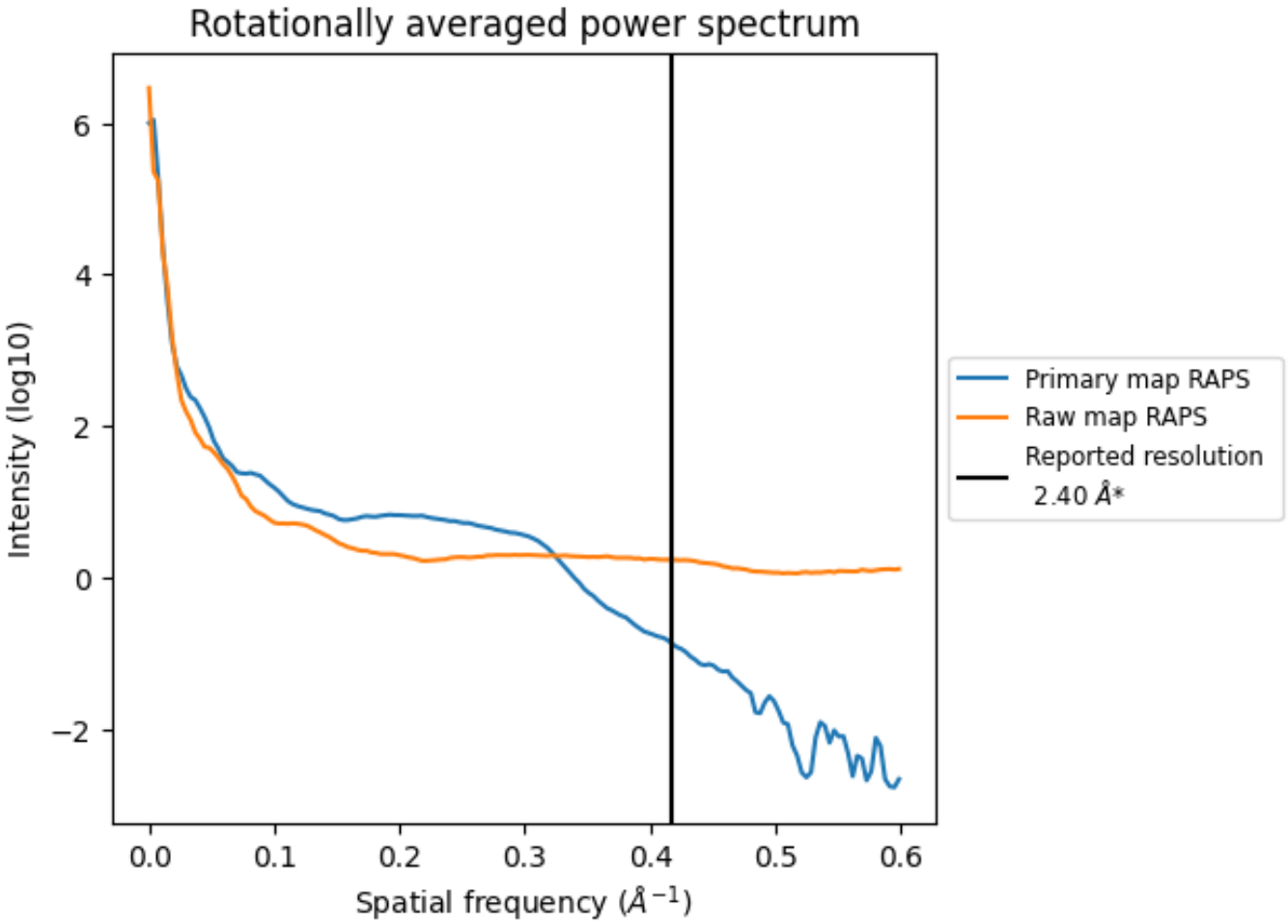
7.2 Volume estimate



The volume at the recommended contour level is 1859 nm^3; this corresponds to an approximate mass of 1680 kDa.

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

7.3 Rotationally averaged power spectrum (i)

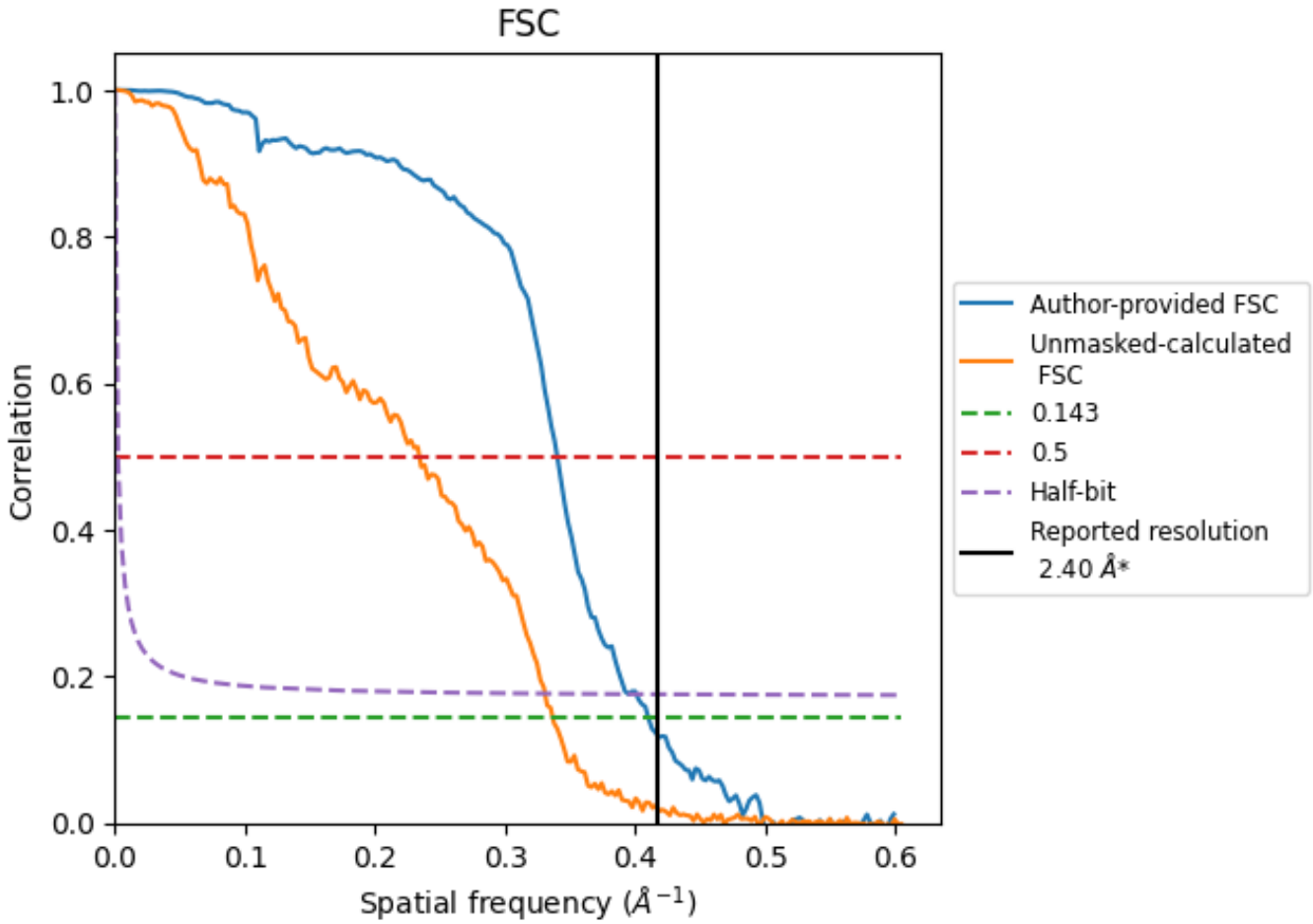


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8.2 Resolution estimates (i)

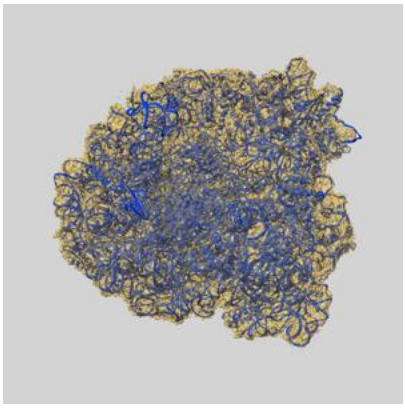
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.44	2.94	2.49
Unmasked-calculated*	2.97	4.27	3.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.97 differs from the reported value 2.4 by more than 10 %

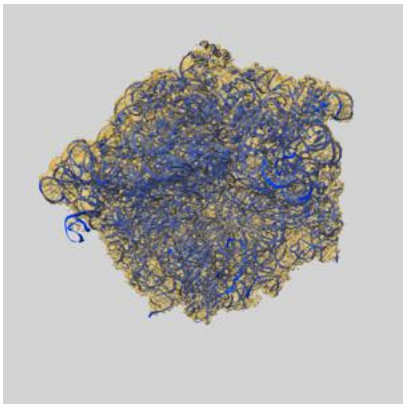
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12694 and PDB model 7O1A. Per-residue inclusion information can be found in section 3 on page 17.

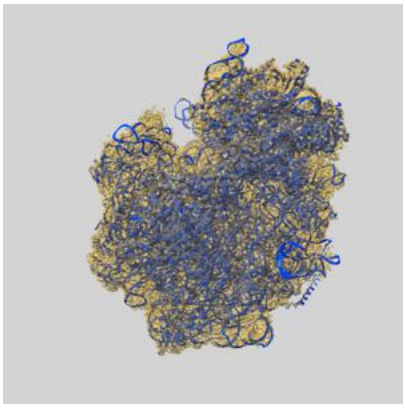
9.1 Map-model overlay



X



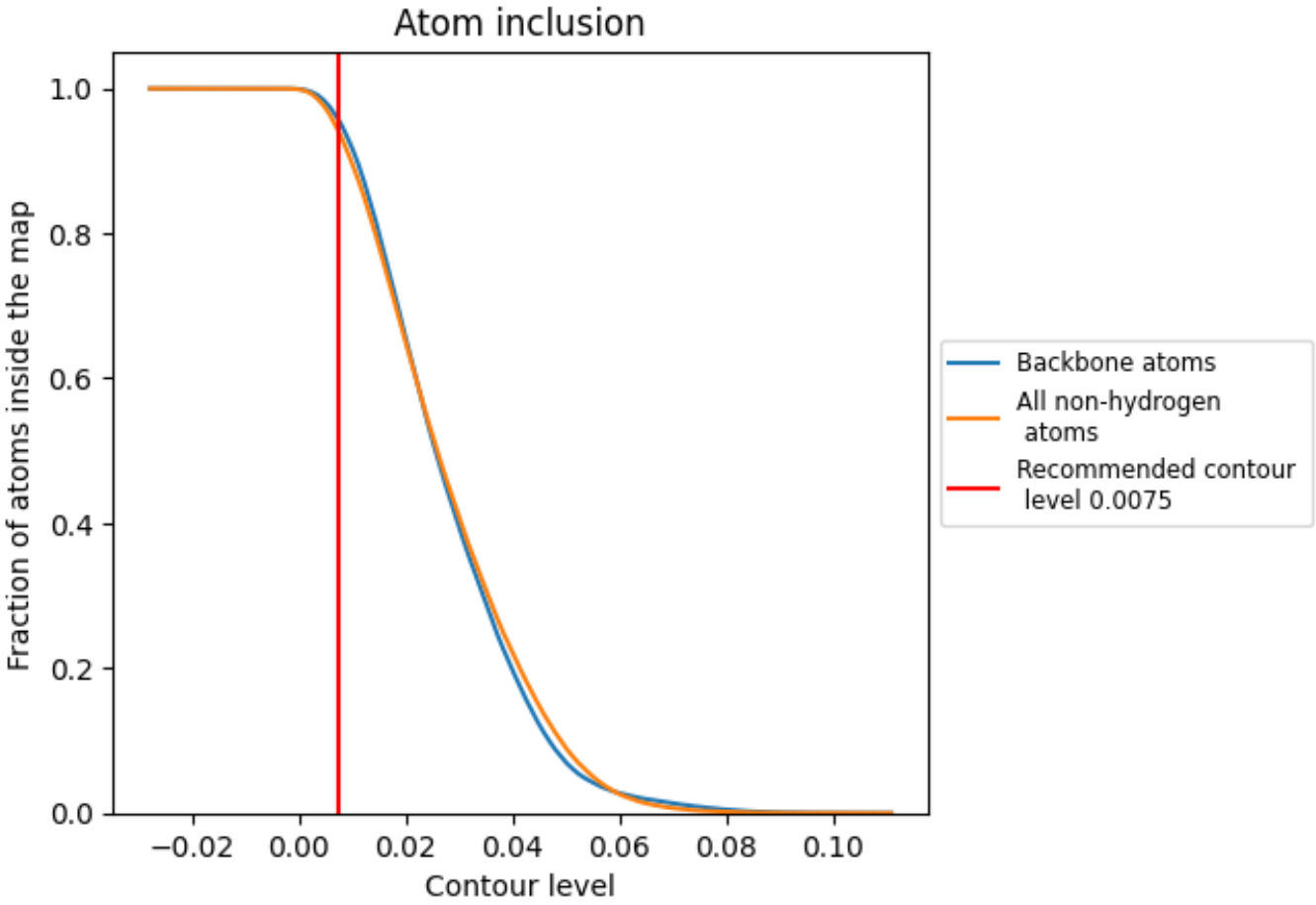
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.