Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:35 pm GMT

PDB ID	:	5JTE
EMDB ID	:	EMD-8175
Title	:	Cryo-EM structure of an ErmBL-stalled ribosome in complex with A-, P-, and E-tRNA
Authors	:	Arenz, S.; Bock, L.V.; Graf, M.; Innis, C.A.; Beckmann, R.; Grubmueller, H.; Vaiana, A.C.; Wilson, D.N.
Deposited on	:	2016-05-09
Resolution	:	3.60 Å(reported)
Based on initial model	:	5AFI

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

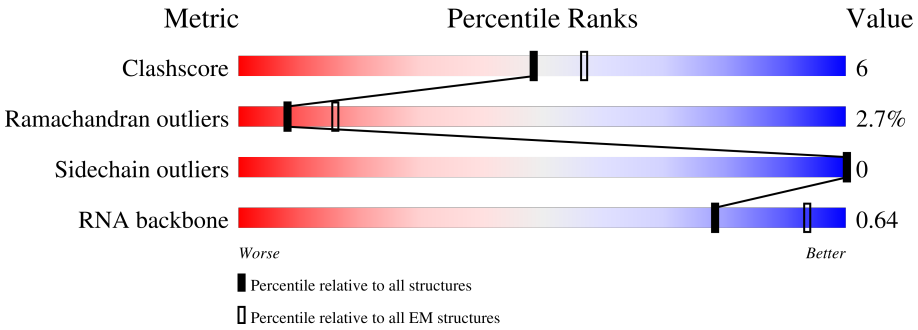
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.60 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	1539	67% 53% 35% 11% ·
2	AB	240	91% 65% 25% · 9%
3	AC	233	88% 64% 24% 12%
4	AD	206	100% 55% 43% ·
5	AE	167	87% 66% 22% · 10%
6	AF	135	73% 56% 18% · 26%
7	AG	179	84% 66% 18% 16%

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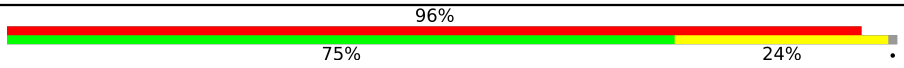
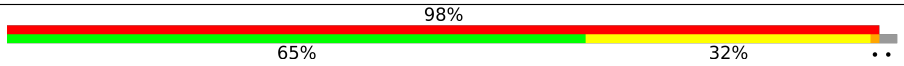
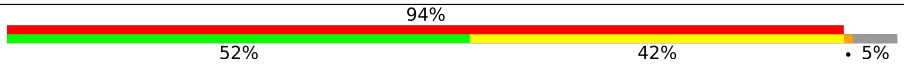
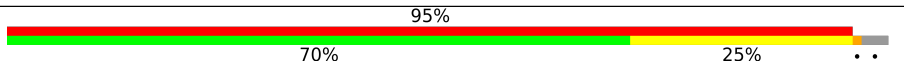
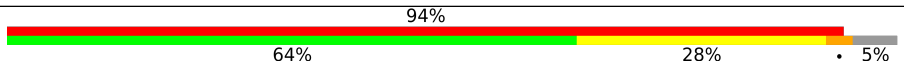
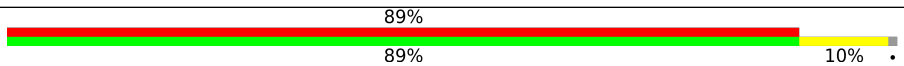
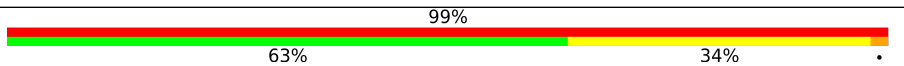
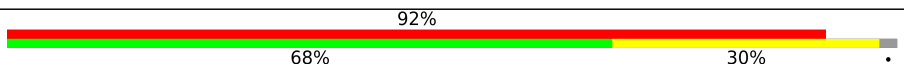
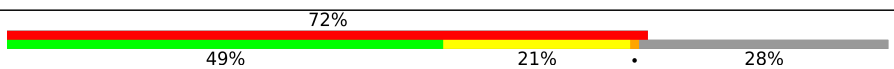
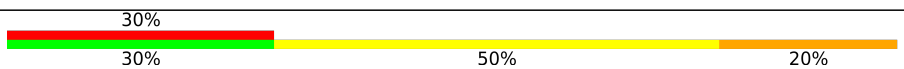
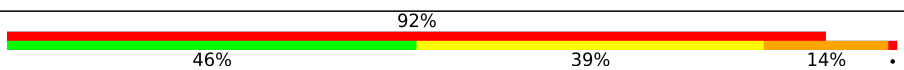
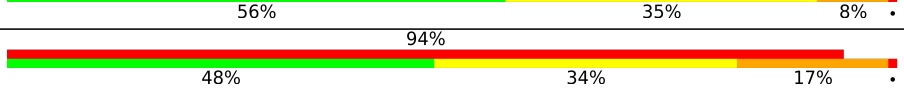
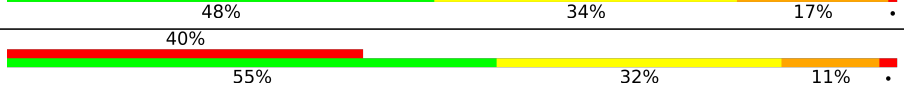
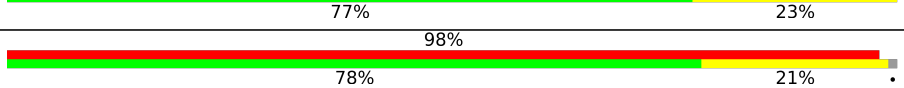
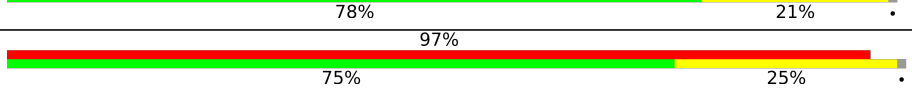
Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	10	
23	AW	74	
24	AX	77	
25	AY	71	
26	BA	2897	
27	BB	120	
28	BC	273	
29	BD	209	
30	BE	201	
31	BF	179	
32	BG	177	

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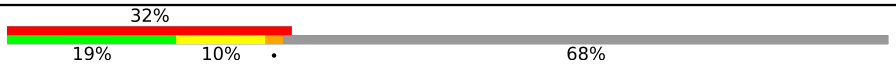
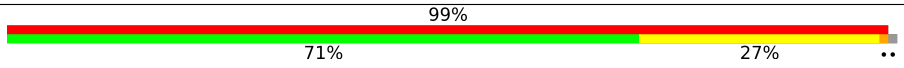
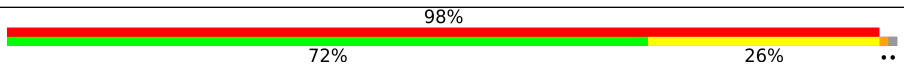
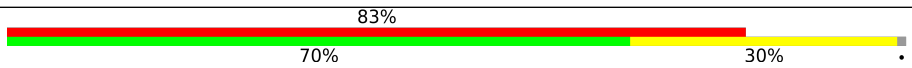
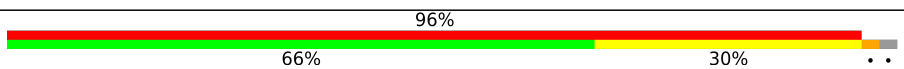
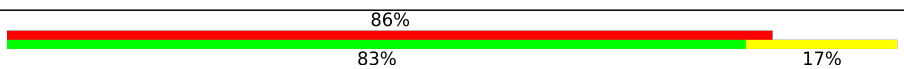
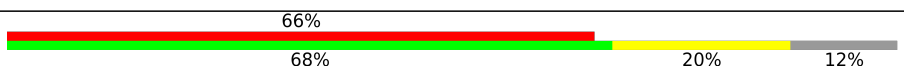
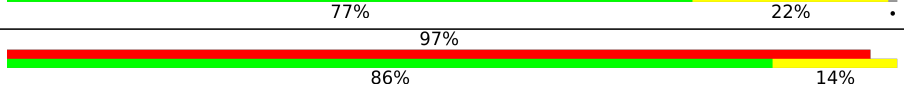
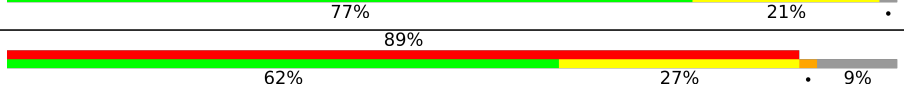
Mol	Chain	Length	Quality of chain
33	BH	149	
34	BI	142	
35	BJ	142	
36	BK	123	
37	BL	144	
38	BM	136	
39	BN	127	
40	BO	117	
41	BP	115	
42	BQ	118	
43	BR	103	
44	BS	110	
45	BT	100	
46	BU	104	
47	BV	94	
48	BW	85	
49	BX	78	
50	BY	63	
51	BZ	59	
52	B0	57	
53	B1	55	
54	B2	46	
55	B3	65	
56	B4	38	
57	B5	9	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 146760 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	1539	33015	14725	6052	10699	1539	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	218	1704	1081	305	311	7	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	150	1105	687	211	201	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	100	817	515	148	148	6	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	98	Total	C	N	O	S	0	0
			786	493	150	142	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
			955	590	196	165	4		

- 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	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- 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
			710	437	143	129	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	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0
			218	98	44	66	10		

- Molecule 23 is a RNA chain called A-site Lysine tRNA Lysine.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0
			1593	716	280	522	73	2		

- Molecule 24 is a RNA chain called P-site tRNA Aspartate.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	77	Total	C	N	O	P	S	0	0
			1656	741	290	547	77	1		

- Molecule 25 is a RNA chain called E-site tRNA Valine.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	AY	71	Total	C	N	O	P	S	0	0
			1525	682	276	496	70	1		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BA	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BH	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BO	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	75	Total 569	C 353	N 113	O 102	S 1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

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

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 54 is a protein called 50S ribosomal protein L34.

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

- Molecule 55 is a protein called 50S ribosomal protein L35.

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

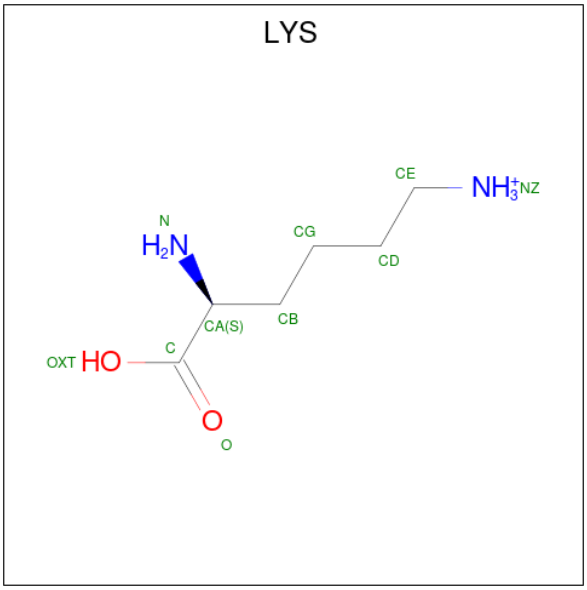
- Molecule 56 is a protein called 50S ribosomal protein L36.

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

- Molecule 57 is a protein called ErmBL.

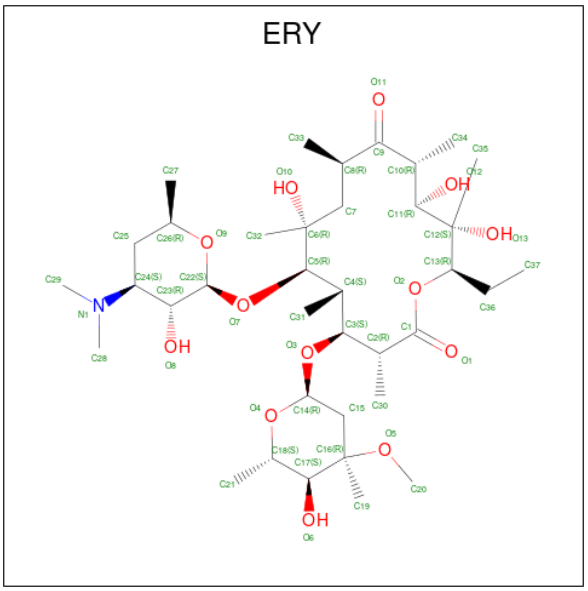
Mol	Chain	Residues	Atoms					AltConf	Trace
57	B5	9	Total	C	N	O	S	0	0
			74	46	14	13	1		

- Molecule 58 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
58	AW	1	Total	C	N	O	0
			9	6	2	1	

- Molecule 59 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



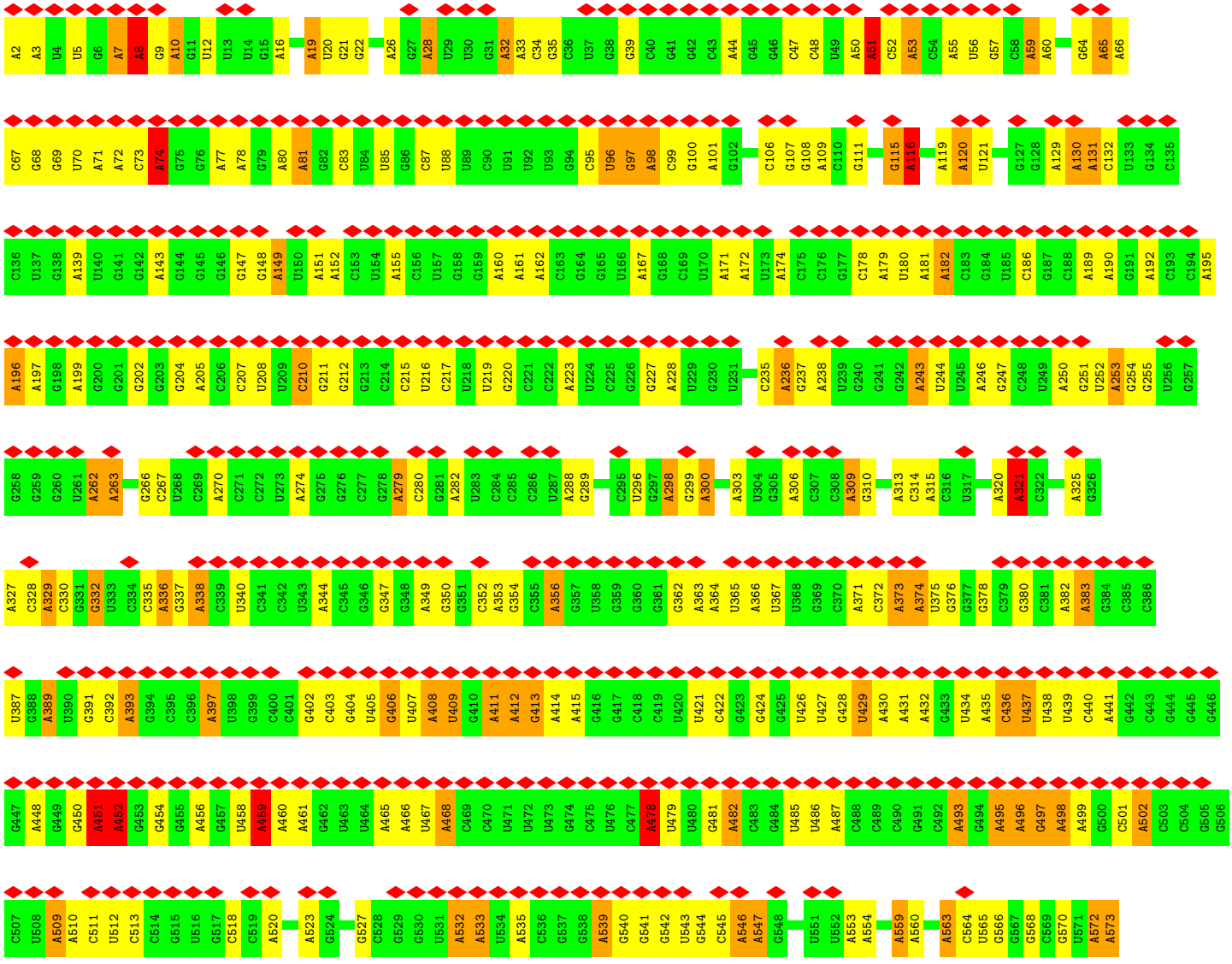
Mol	Chain	Residues	Atoms				AltConf
59	BA	1	Total	C	N	O	0
			51	37	1	13	

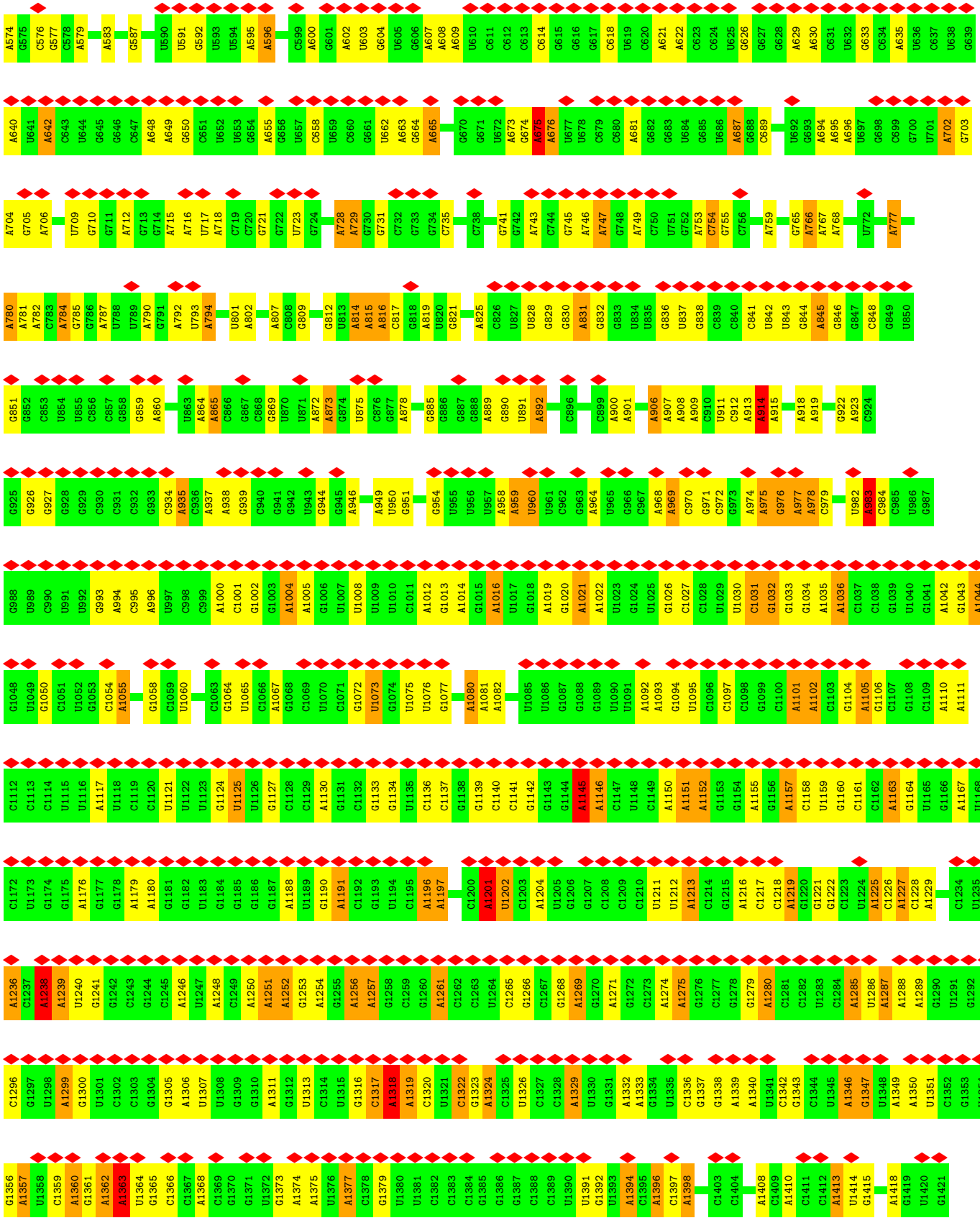
3 Residue-property plots (i)

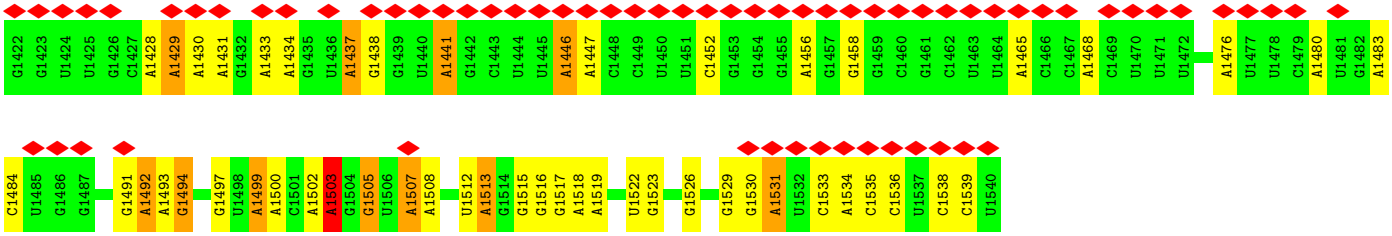
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 16S ribosomal RNA

Chain AA:

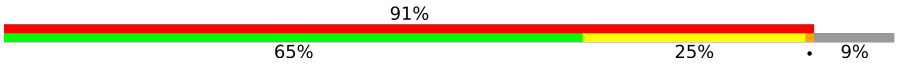


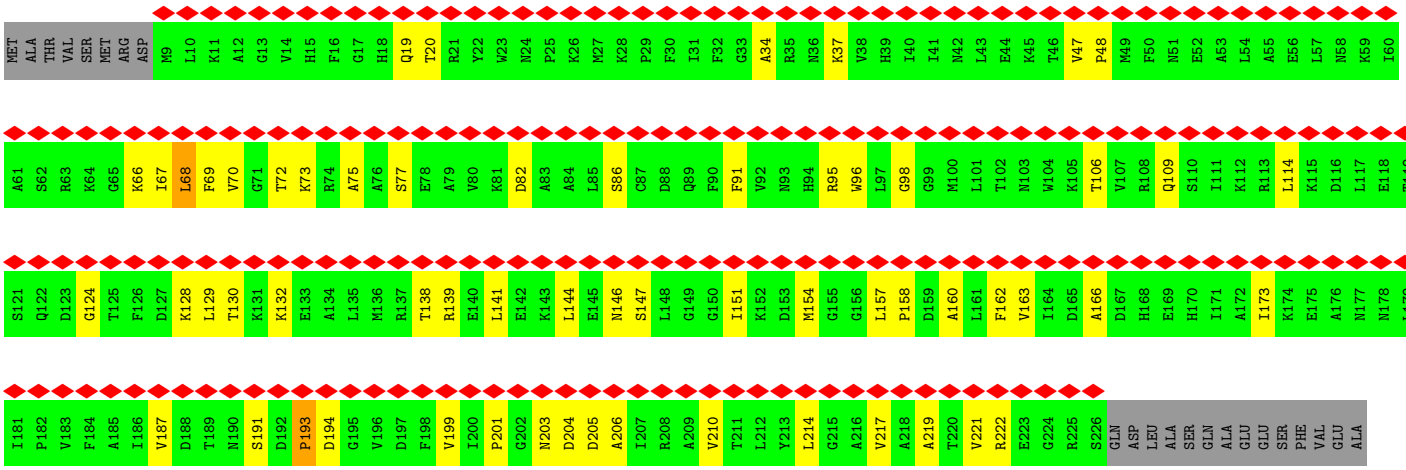

A574 G575 C576 G577 C578 A579 A583 G587 U590 U591 G592 U593 U594 A595 A596 C599 A600 G601 A602 U603 G604 U605 G606 A607 A608 A609 U610 C611 C612 C613 C614 G615 G616 G617 C618 U619 C620 A621 A622 C623 C624 U625 G626 G627 G628 A629 A630 C631 U632 G633 C634 A635 U636 C637 U638 G639
A640 U641 A642 C643 U644 G645 G646 C647 A648 A649 G650 C651 U652 U653 G654 A655 G656 U657 C658 U659 C660 G661 U662 A663 G664 A665 G670 G671 U672 A673 G674 A675 A676 U677 U678 C679 C680 A681 G682 G683 U684 G685 U686 A687 G688 C689 U692 G693 A694 A695 A696 U697 G698 C699 G700 U701 A702 G703
A704 G705 A706 U709 G710 G711 A712 G713 G714 A715 A716 U717 A718 C719 C720 G721 G722 U723 G724 A728 A729 G730 G731 C732 G733 G734 C735 C738 G741 G742 A743 C744 G745 A746 A747 G748 A749 C750 U751 G752 A753 C754 G755 C756 A759 G765 A766 A767 A768 U772 A777
A780 A781 A782 C783 A784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 U801 A802 A807 C808 G809 G812 U813 A814 A815 A816 C817 G818 A819 U820 G821 A825 C826 U827 U828 G829 G830 A831 G832 G833 U834 U835 G836 U837 G838 C839 C840 C841 U842 U843 G844 A845 G846 G847 C848 G849 U850
G851 G852 C853 U854 U855 C856 C857 G858 G859 A860 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 U875 C876 G877 A878 G885 G886 G887 G888 A889 G890 U891 A892 C896 C899 A900 A901 A906 A907 A908 A909 C910 U911 C912 U913 A914 A915 A918 A919 G922 A923 C924
G925 G926 G927 G928 G929 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G944 G945 A946 A949 U950 G951 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 U965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 U982 A983 C984 C985 U986 G987
G988 U989 C990 U991 U992 G993 A994 C995 A996 U997 C998 C999 A1000 C1001 G1002 G1003 A1004 A1005 G1006 U1007 U1008 U1009 U1010 C1011 A1012 G1013 A1014 G1015 A1016 U1017 G1018 A1019 G1020 A1021 A1022 U1023 G1024 U1025 G1026 C1027 C1028 U1029 U1030 C1031 G1032 G1033 G1034 A1035 A1036 C1037 C1038 G1039 U1040 G1041 A1042 G1043 A1044 C1045 A1046 G1047
G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 G1058 C1059 U1060 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 U1075 U1076 G1077 A1080 A1081 A1082 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111
C1112 C1113 C1114 U1115 U1116 A1117 U1118 C1119 C1120 U1121 U1122 U1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 C1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 A1145 A1146 C1147 U1148 C1149 A1150 A1151 A1152 G1153 G1154 A1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 A1163 G1164 U1165 G1166 A1167 U1168 A1169 A1170 A1171
C1172 U1173 G1174 U1175 A1176 G1177 C1178 A1179 A1180 G1181 G1182 U1183 G1184 C1185 G1186 G1187 A1188 U1189 G1190 A1191 C1192 G1193 U1194 C1195 A1196 A1197 C1200 A1201 U1202 C1203 A1204 U1205 G1206 C1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 A1216 C1217 C1218 A1219 G1220 G1221 G1222 C1223 U1224 A1225 C1226 A1227 C1228 A1229 C1234 U1235
A1236 C1237 A1238 A1239 U1240 G1241 G1242 C1243 G1244 C1245 A1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 A1254 G1255 A1256 A1257 G1258 C1259 G1260 A1261 C1262 C1263 U1264 C1265 G1266 C1267 G1268 A1269 G1270 A1271 G1272 C1273 A1274 A1275 G1276 C1277 G1278 C1279 A1280 C1281 C1282 U1283 C1284 A1285 U1286 A1287 A1288 A1289 G1290 U1291 C1292 C1293 G1294 U1295
C1296 G1297 U1298 A1299 G1300 U1301 C1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 A1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 U1321 C1322 G1323 A1324 C1325 U1326 C1327 C1328 A1329 U1330 G1331 A1332 A1333 G1334 U1335 C1336 G1337 G1338 A1339 A1340 U1341 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 U1354 G1355
G1356 A1357 U1358 C1359 A1360 G1361 A1362 A1363 U1364 G1365 C1366 C1367 A1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378 G1379 U1380 U1381 C1382 C1383 C1384 G1385 G1386 G1387 C1388 C1389 U1390 U1391 G1392 U1393 A1394 C1395 A1396 C1397 A1398 C1403 C1404 A1408 C1409 A1410 C1411 C1412 A1413 U1414 G1415 A1418 G1419 U1420 G1421



• Molecule 2: 30S ribosomal protein S2

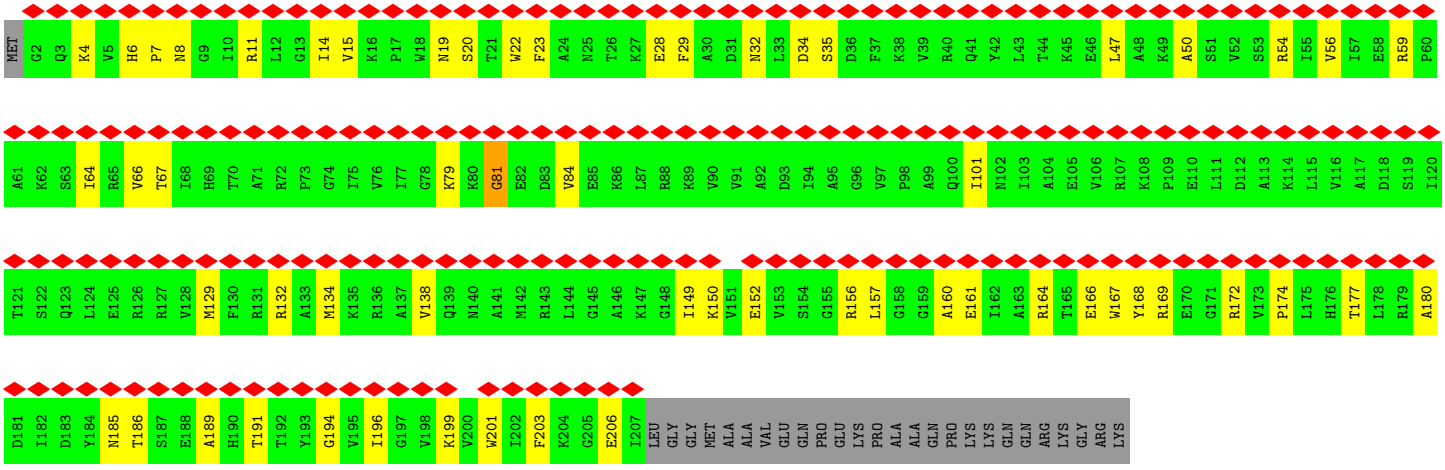
Chain AB:





• Molecule 3: 30S ribosomal protein S3

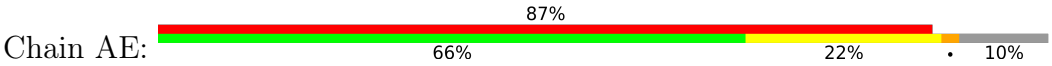
Chain AC:

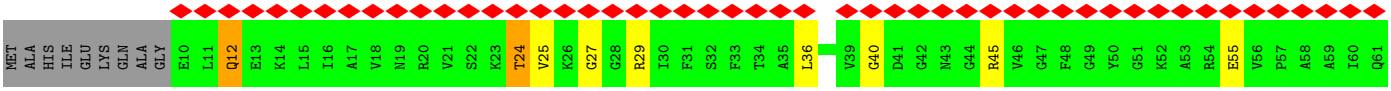


• Molecule 4: 30S ribosomal protein S4

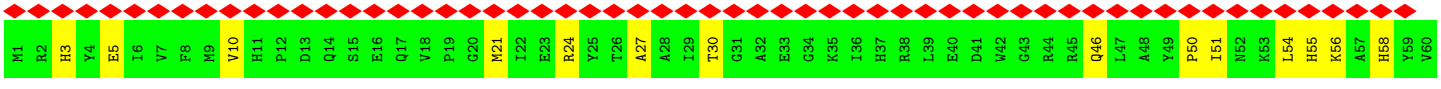
Chain AD:

• Molecule 5: 30S ribosomal protein S5

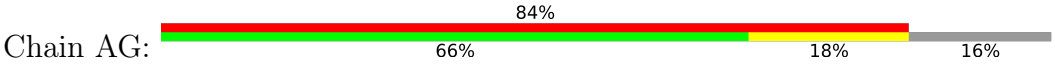


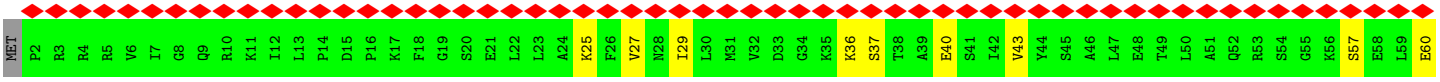


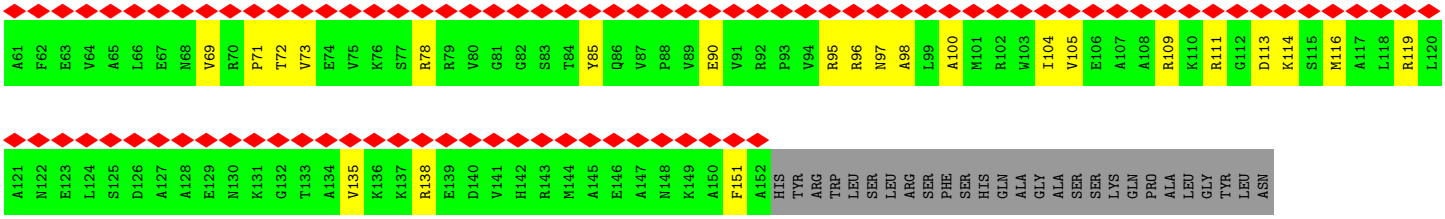
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

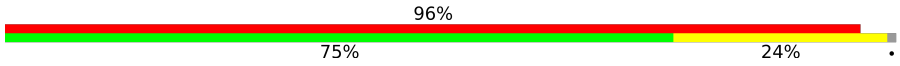


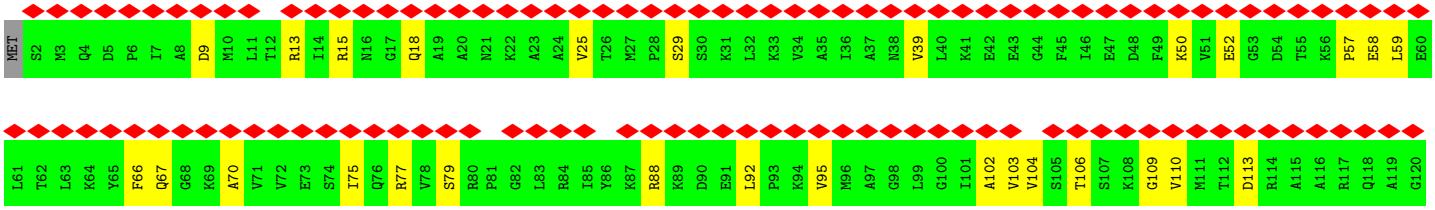




• Molecule 8: 30S ribosomal protein S8

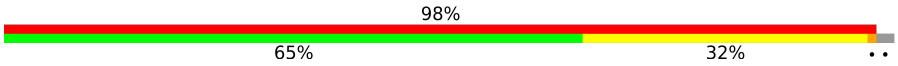
Chain AH:

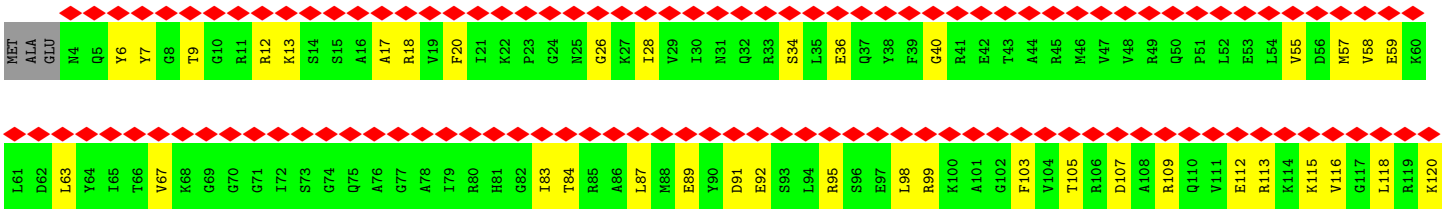




• Molecule 9: 30S ribosomal protein S9

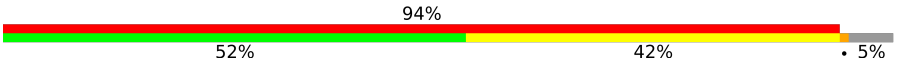
Chain AI:

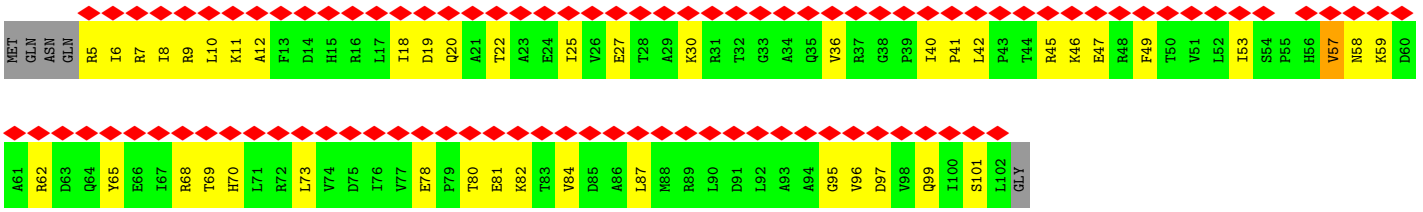




• Molecule 10: 30S ribosomal protein S10

Chain AJ:

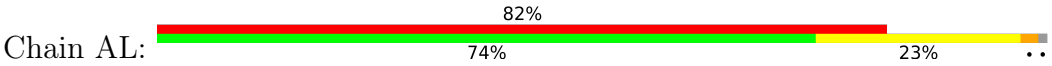


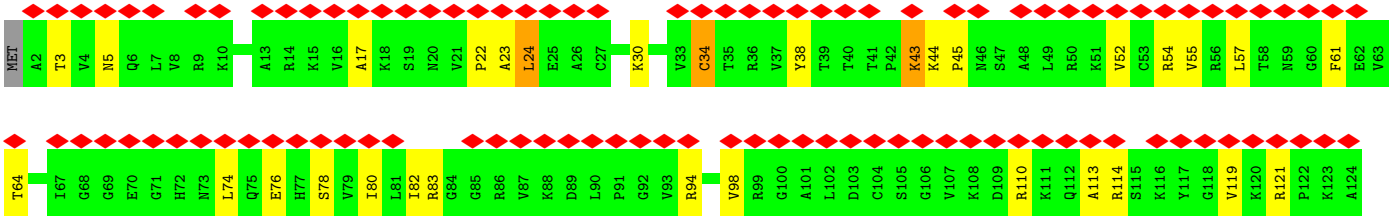


• Molecule 11: 30S ribosomal protein S11

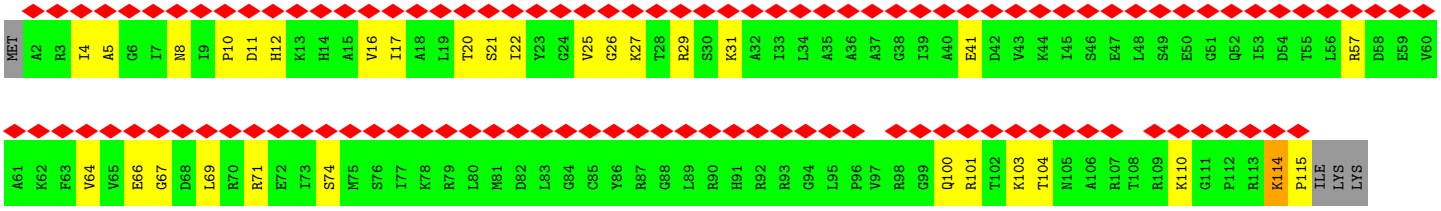
Chain AK:

• Molecule 12: 30S ribosomal protein S12

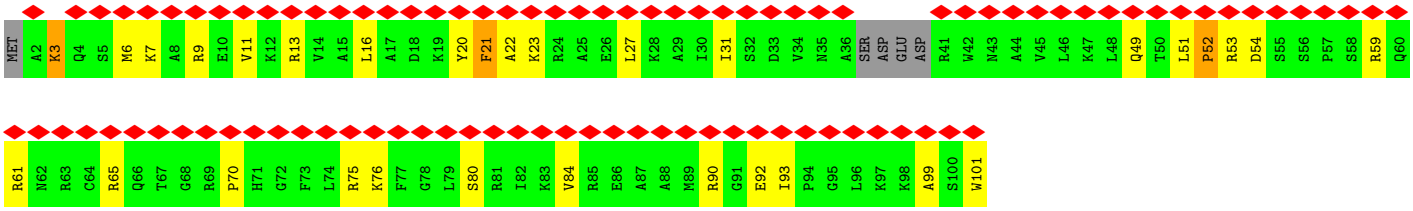




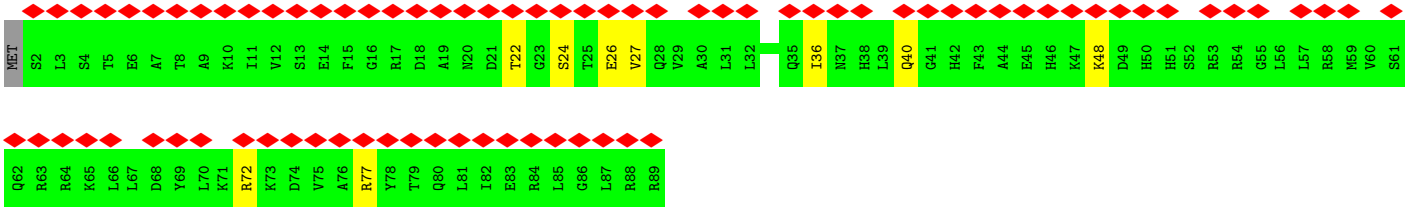
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14

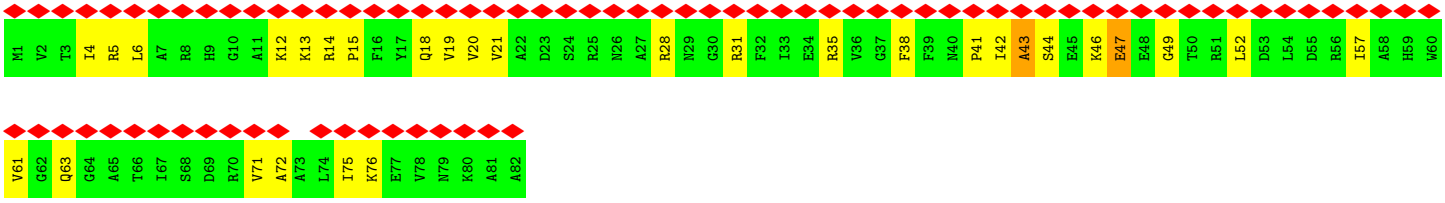


• Molecule 15: 30S ribosomal protein S15



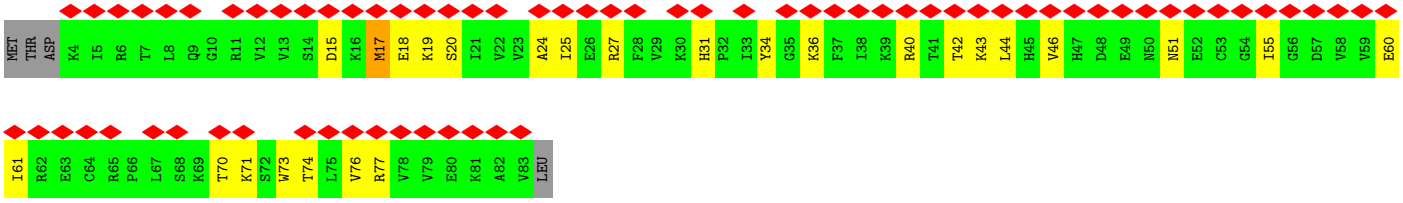
• Molecule 16: 30S ribosomal protein S16

Chain AP:



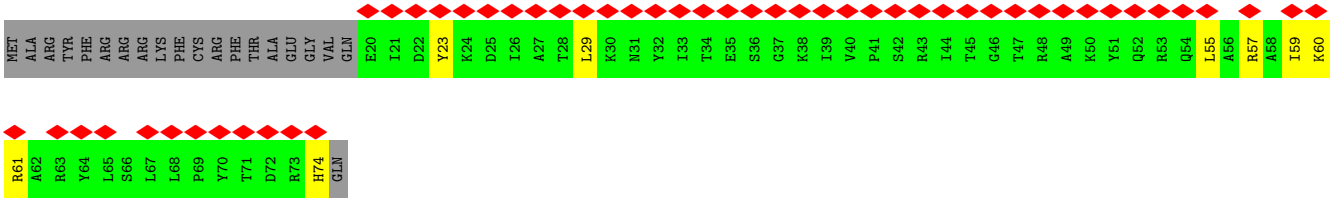
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



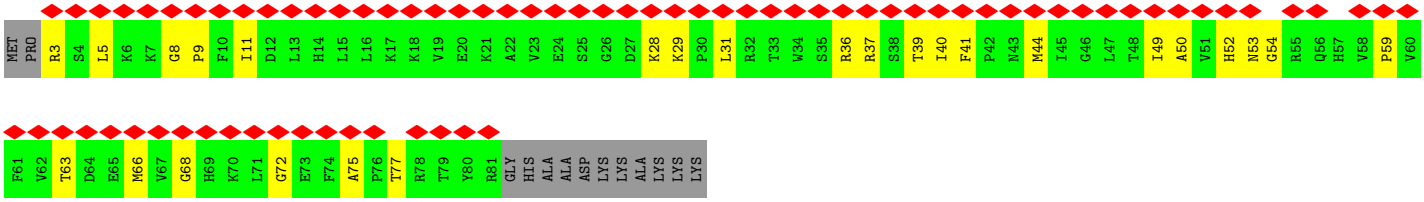
• Molecule 18: 30S ribosomal protein S18

Chain AR:



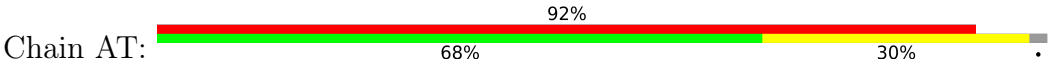
• Molecule 19: 30S ribosomal protein S19

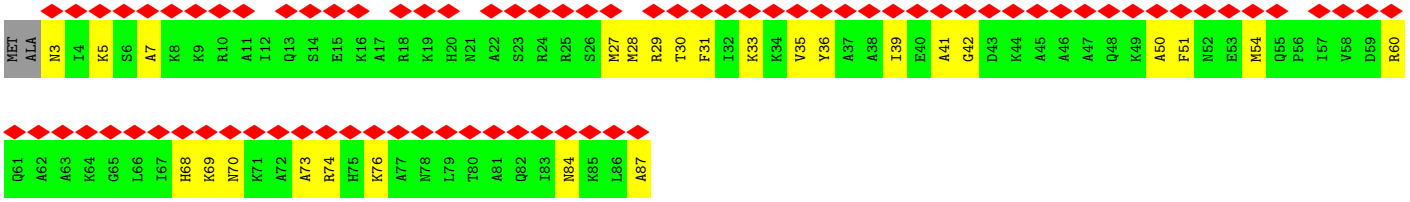
Chain AS:



• Molecule 20: 30S ribosomal protein S20

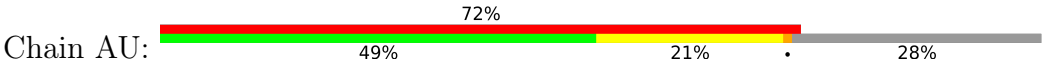
Chain AT:

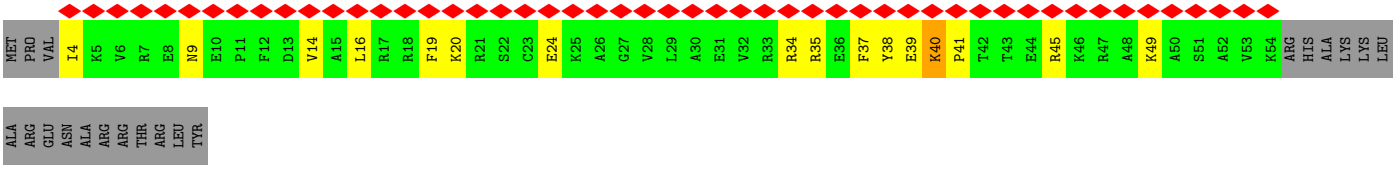




• Molecule 21: 30S ribosomal protein S21

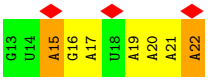
Chain AU:





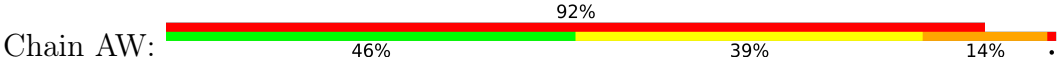
• Molecule 22: mRNA

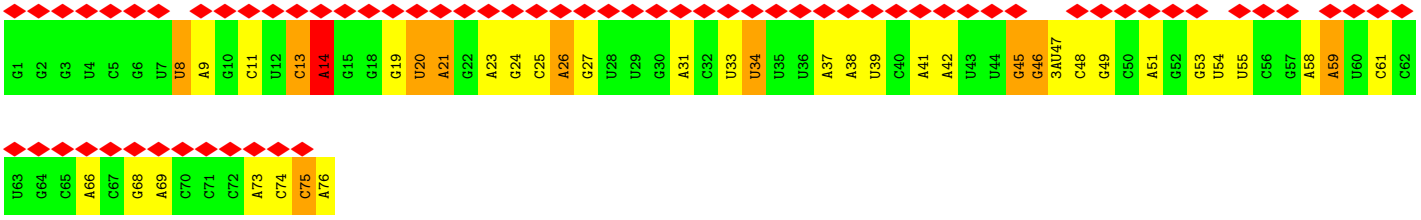
Chain AV:



• Molecule 23: A-site Lysine tRNA Lysine

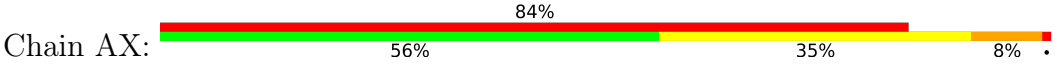
Chain AW:

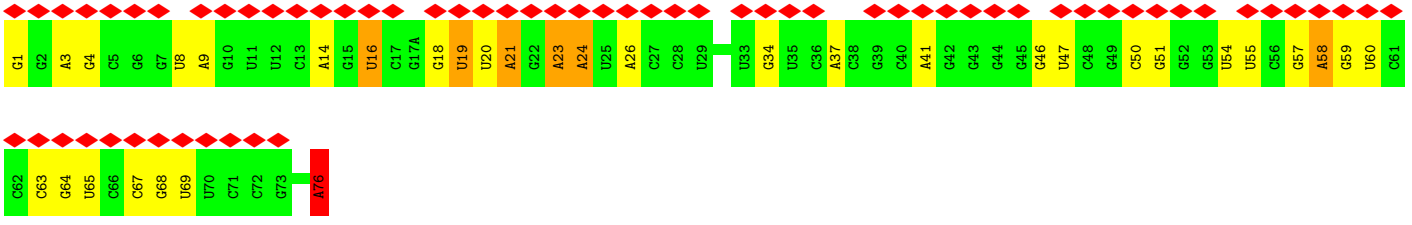




• Molecule 24: P-site tRNA Aspartate

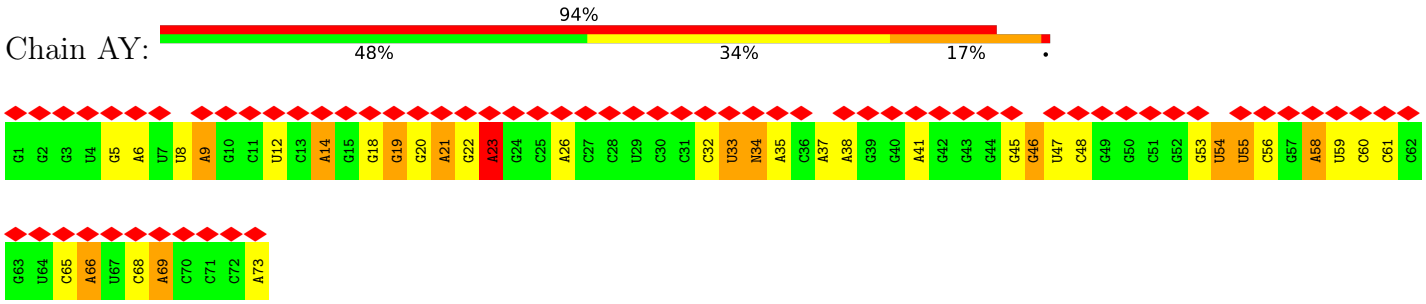
Chain AX:





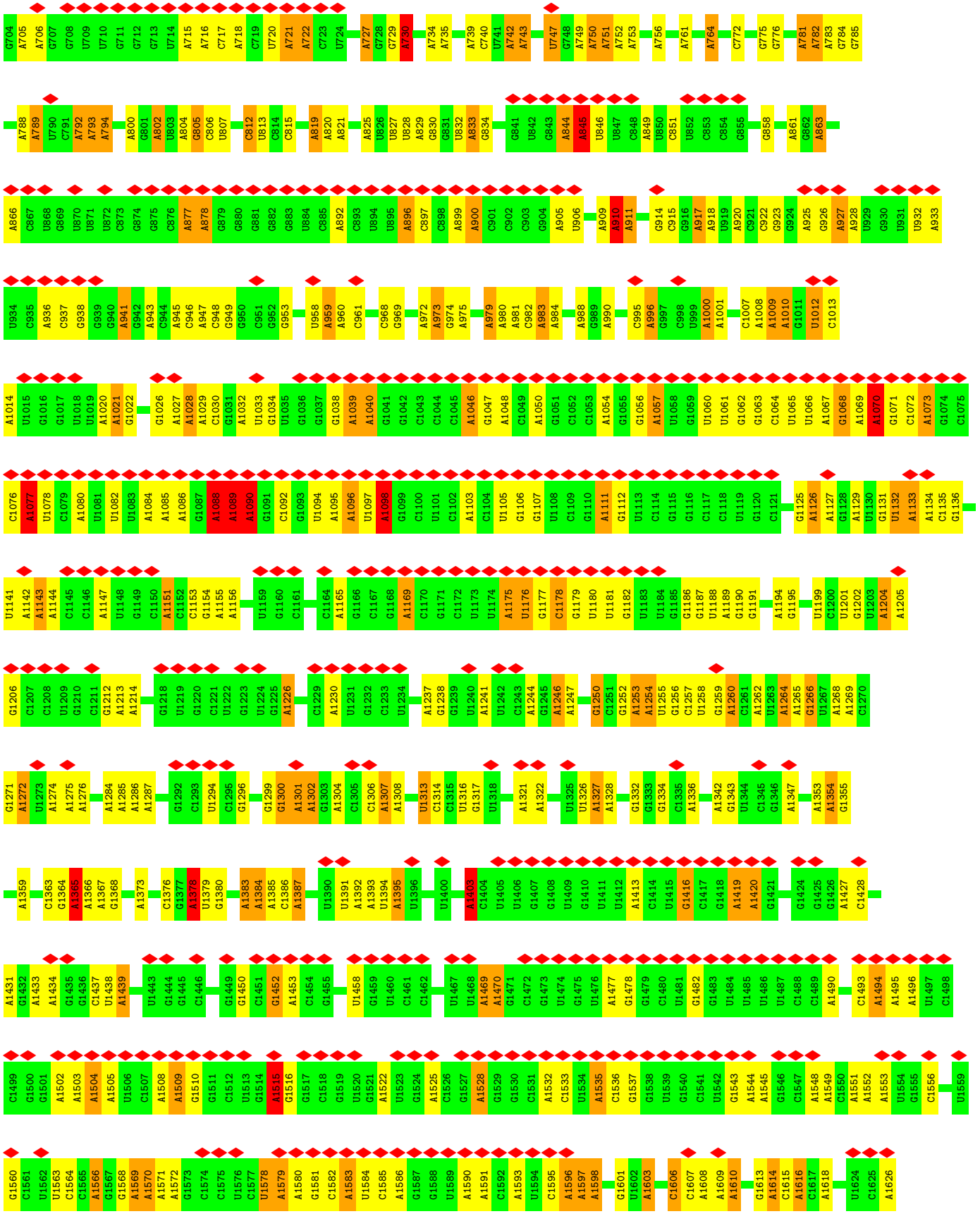
• Molecule 25: E-site tRNA Valine

Chain AY:



• Molecule 26: 23S ribosomal RNA

Chain BA:


G704 A705 A706 G707 G708 U709 U710 G711 G712 G713 U714 A715 A716 C717 A718 C719 U720 A721 A722 C723 U724 A727 G728 G729 A730 A734 A735 A739 C740 U741 A742 A743 U747 G748 A749 A750 A751 A752 A753 A756 A761 A764 C772 G775 G776 A781 A782 A783 G784 G785
A788 A789 U790 C791 A792 A793 A794 A800 G801 A802 U803 A804 G805 C806 U807 C812 U813 C814 C815 A819 A820 A821 A825 U826 U827 U828 A829 G830 G831 U832 A833 G834 G841 U842 G843 A844 A845 U846 U847 C848 A849 U850 C851 U852 C853 C854 G855 G858 A861 G862 A863
A866 C867 U868 G869 U870 U871 U872 C873 G874 G875 C876 A877 A878 G879 G880 G881 G882 G883 U884 C885 A892 C893 U894 U895 A896 C897 C898 A899 A900 C901 C902 C903 G904 A905 U906 A909 A910 A911 G914 C915 G916 A917 A918 U919 A920 C921 C922 G923 G924 A925 G926 A927 A928 U929 G930 U931 U932 A933
U934 C935 A936 C937 G938 G939 G940 A941 G942 A943 C944 A945 C946 A947 C948 G949 G950 C951 G952 G953 U958 A959 A960 C961 C968 G969 A972 A973 G974 A975 A979 A980 A981 C982 A983 A984 A988 G989 A990 C995 A996 G997 C998 U999 A1000 A1001 C1007 A1008 A1009 A1010 G1011 U1012 C1013
A1014 U1015 G1016 G1017 U1018 U1019 A1020 A1021 G1022 G1026 A1027 A1028 A1029 C1030 G1031 A1032 U1033 G1034 U1035 G1036 G1037 G1038 A1039 A1040 G1041 G1042 C1043 C1044 C1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075
C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 G1116 C1117 C1118 U1119 G1120 C1121 G1125 A1126 A1127 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136
U1141 A1142 A1143 A1144 C1145 C1146 A1147 U1148 G1149 C1150 A1151 C1152 C1153 G1154 A1155 A1156 U1159 G1160 C1161 C1164 A1165 G1166 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1185 G1186 G1187 U1188 A1189 G1190 G1191 A1194 G1195 U1199 C1200 U1201 G1202 U1203 A1204 A1205
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G1271 A1272 U1273 A1274 A1275 A1276 A1284 A1285 A1286 A1287 G1292 C1293 U1294 C1295 G1296 G1299 G1300 A1301 A1302 G1303 A1304 C1305 C1306 A1307 A1308 U1313 C1314 C1315 U1316 G1317 U1318 A1321 A1322 U1325 U1326 A1327 A1328 G1332 G1333 G1334 C1335 A1336 A1342 G1343 U1344 C1345 G1346 A1347 A1353 A1354 G1355
A1359 C1363 G1364 A1365 A1366 A1367 G1368 A1373 C1376 G1377 A1378 U1379 G1380 A1383 A1384 A1385 C1386 A1387 U1390 U1391 A1392 A1393 U1394 A1395 U1396 U1400 A1403 C1404 U1405 U1406 G1407 G1408 U1409 G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 G1421 G1424 G1425 G1426 A1427 C1428
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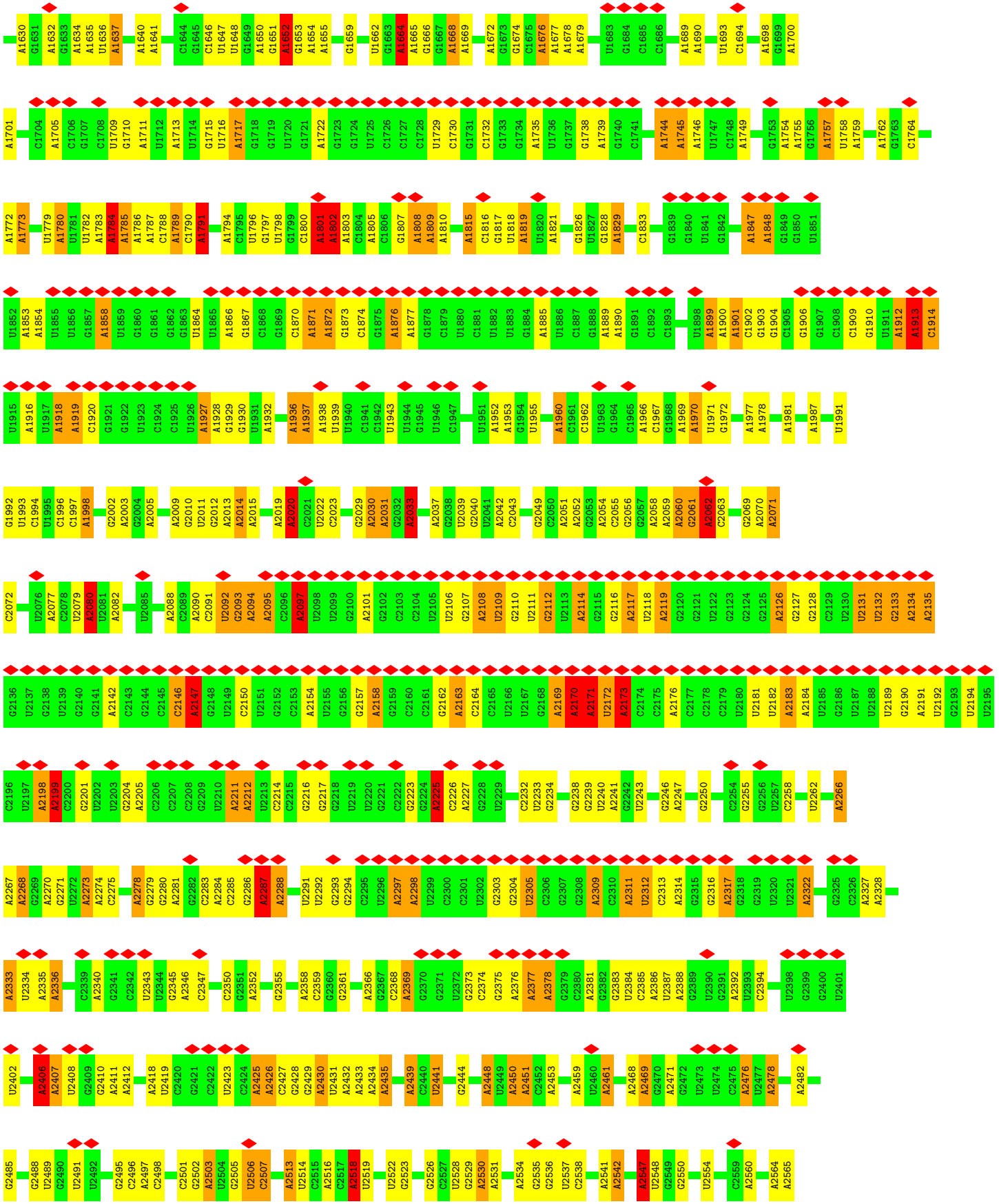
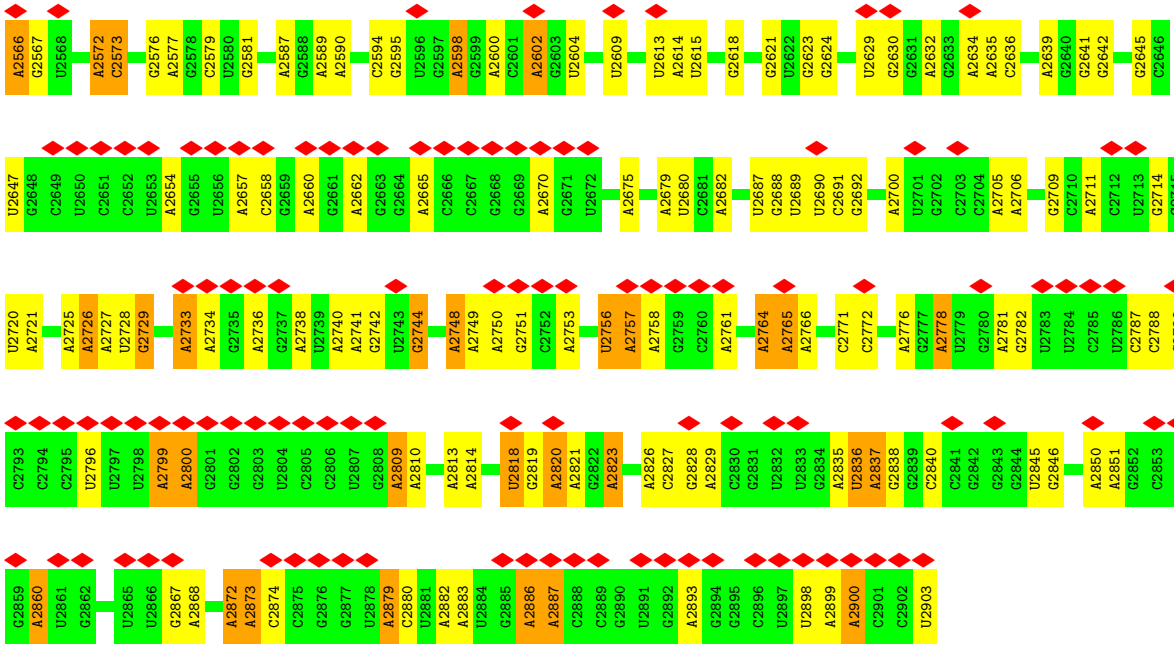
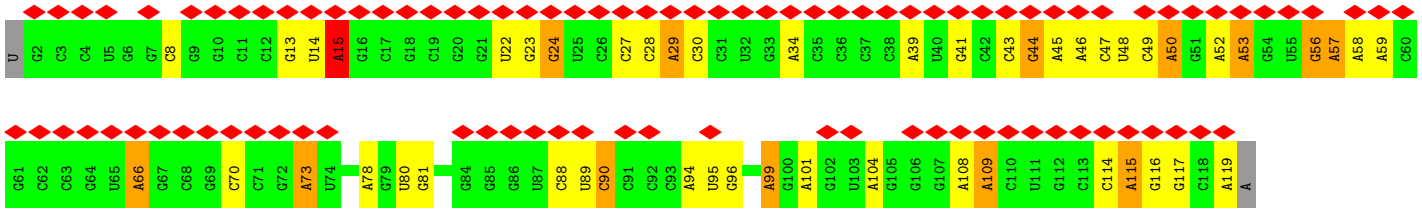
C1499 G1500 G1501 A1502 A1503 A1504 A1505 U1506 C1507 A1508 A1509 G1510 G1511 C1512 U1513 G1514 A1515 G1516 G1517 C1518 G1519 U1520 G1521 A1522 U1523 G1524 A1525 C1526 G1527 A1528 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1544 A1545 G1546 C1547 A1548 A1549 C1550 A1551 A1552 A1553 U1554 G1555 C1556 U1559
G1560 C1561 U1562 A1563 C1564 C1565 A1566 G1567 G1568 A1569 A1570 A1571 A1572 G1573 C1574 C1575 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1591 C1592 A1593 U1594 C1595 A1596 A1597 A1598 G1601 U1602 A1603 C1606 C1607 A1608 A1609 A1610 G1613 A1614 C1615 A1616 C1617 A1618 U1624 C1625 A1626





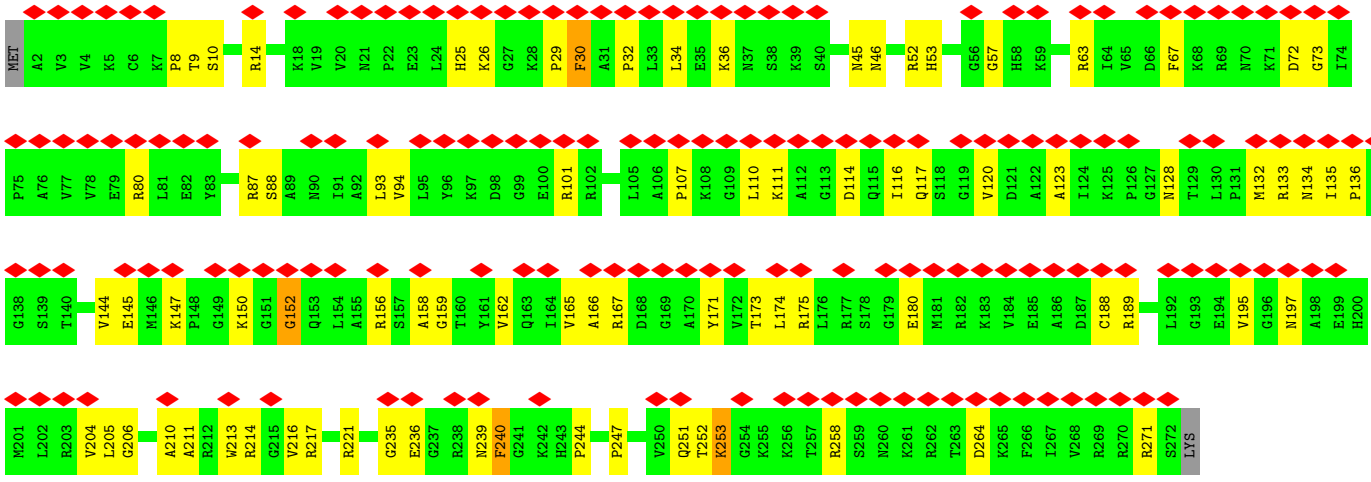
• Molecule 27: 5S ribosomal RNA

Chain BB:



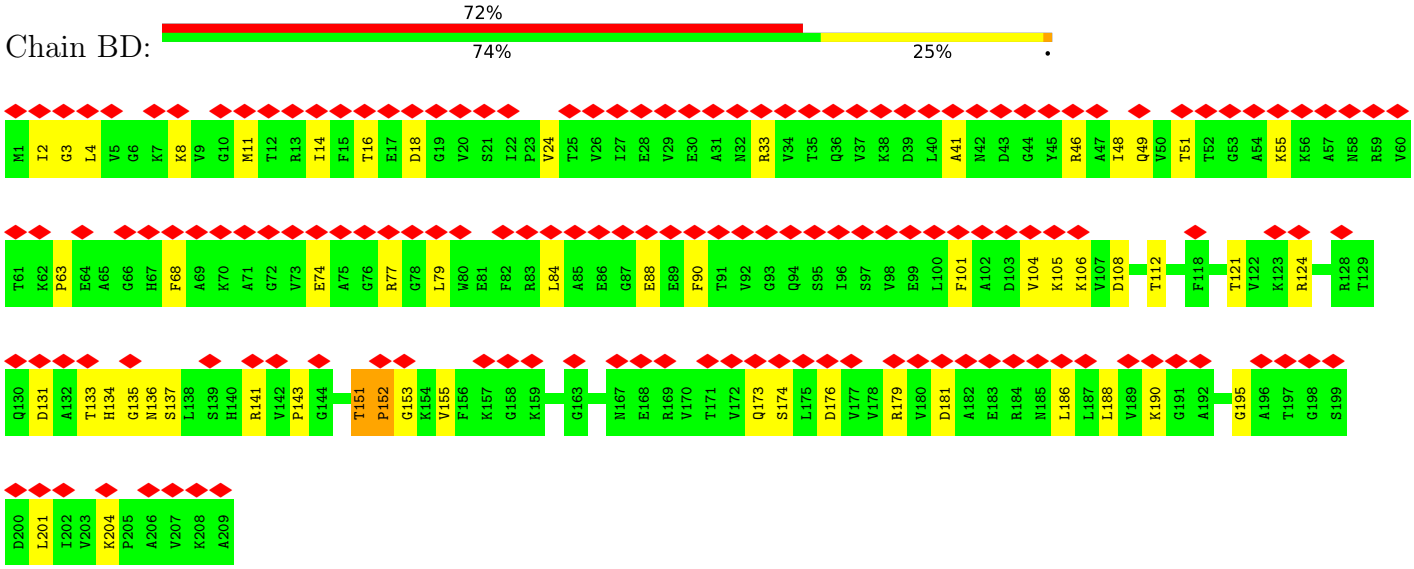
• Molecule 28: 50S ribosomal protein L2

Chain BC:



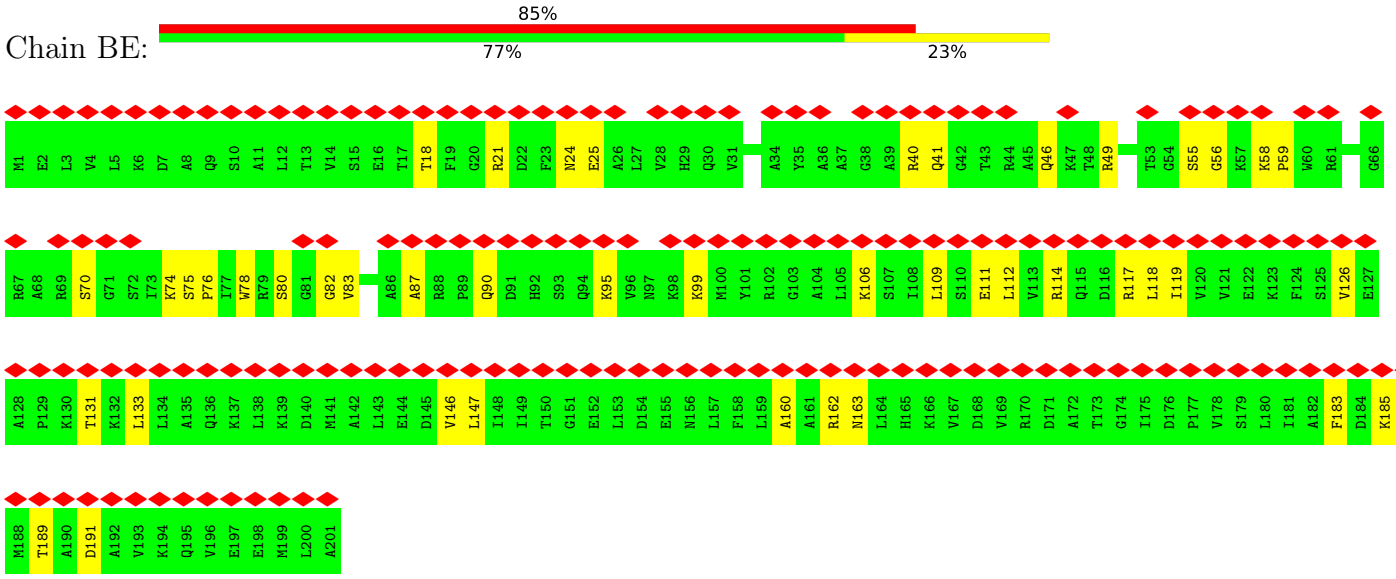
• Molecule 29: 50S ribosomal protein L3

Chain BD:



• Molecule 30: 50S ribosomal protein L4

Chain BE:

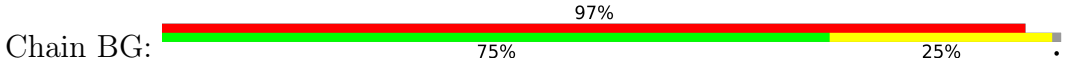


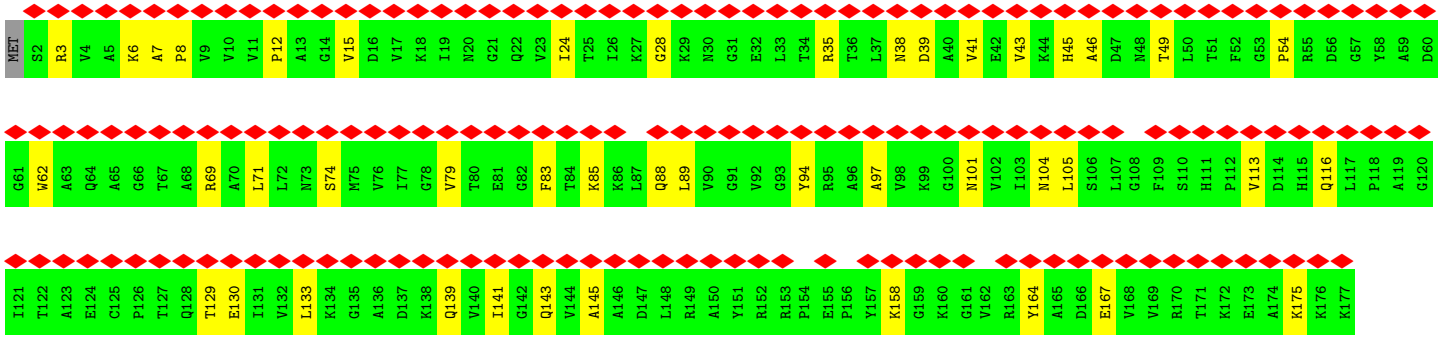
• Molecule 31: 50S ribosomal protein L5

Chain BF:

• Molecule 32: 50S ribosomal protein L6

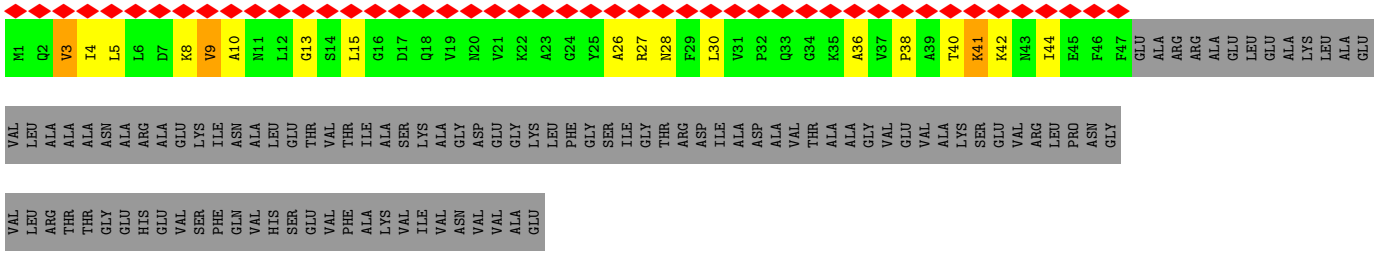
Chain BG:





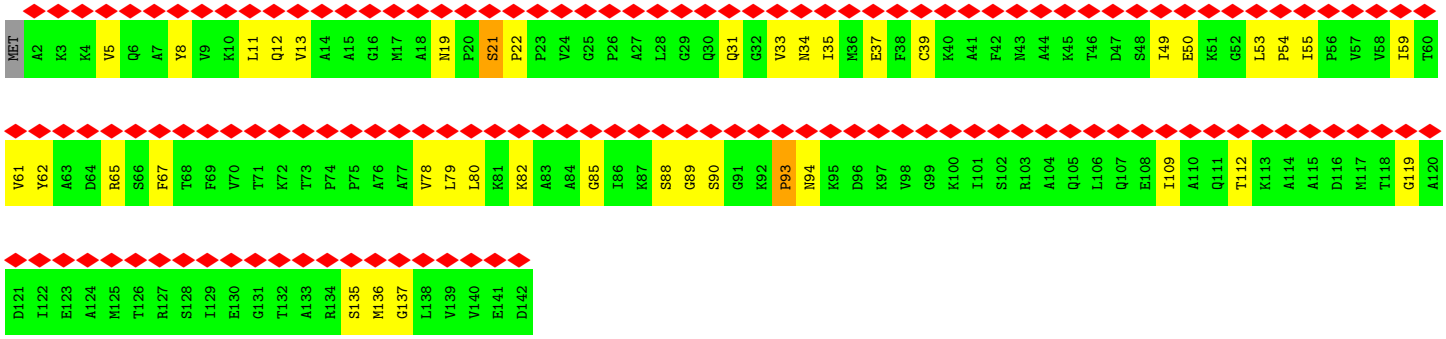
• Molecule 33: 50S ribosomal protein L9

Chain BH:



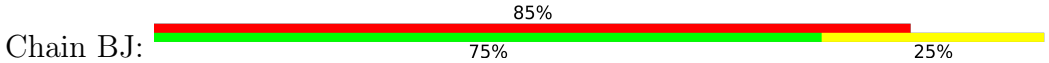
• Molecule 34: 50S ribosomal protein L11

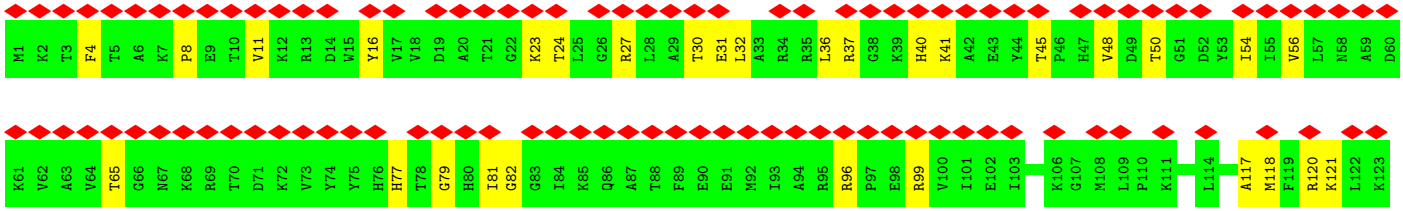
Chain BI:

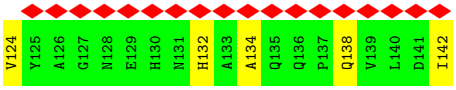


• Molecule 35: 50S ribosomal protein L13

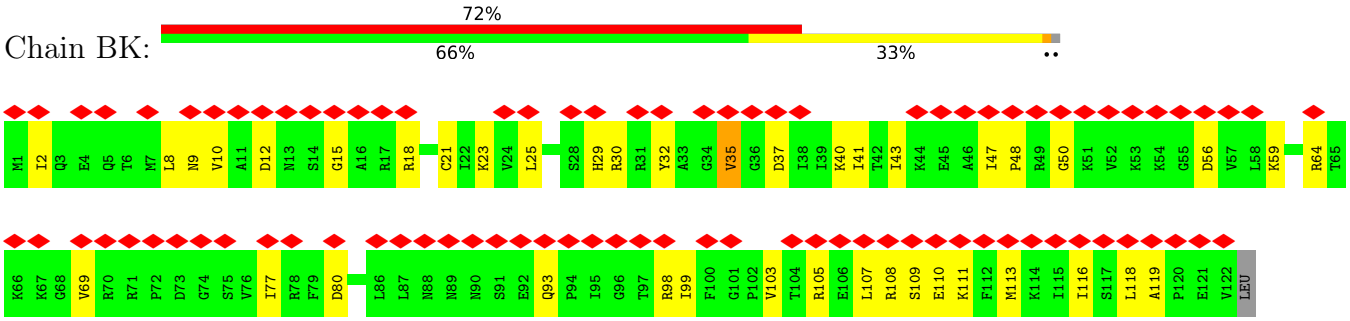
Chain BJ:



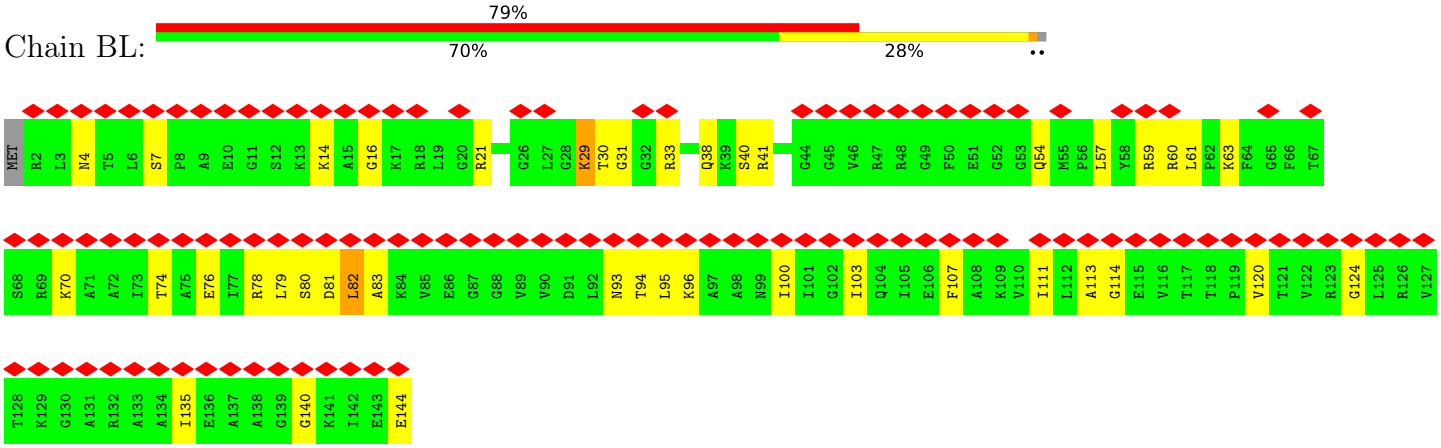




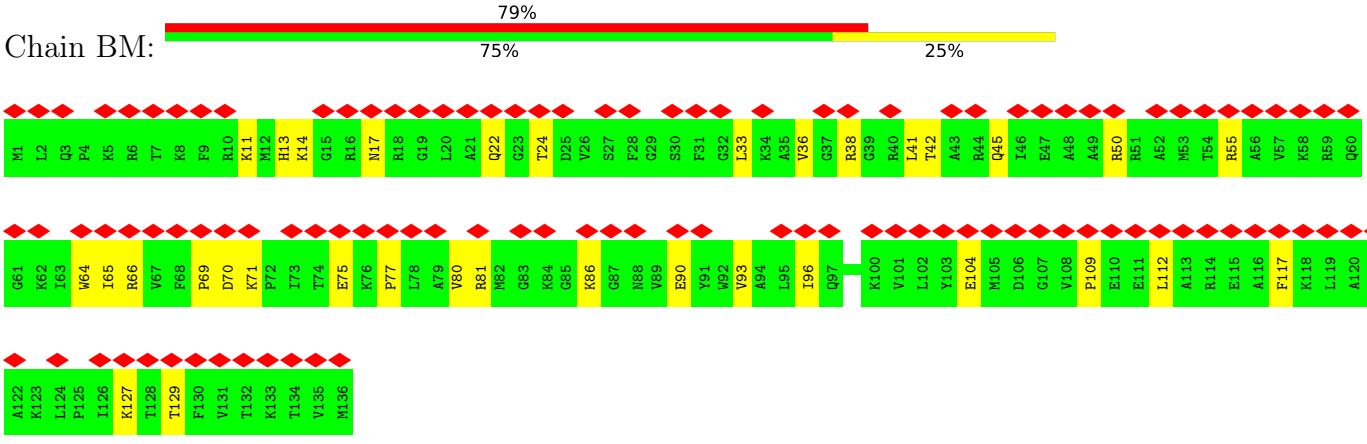
• Molecule 36: 50S ribosomal protein L14



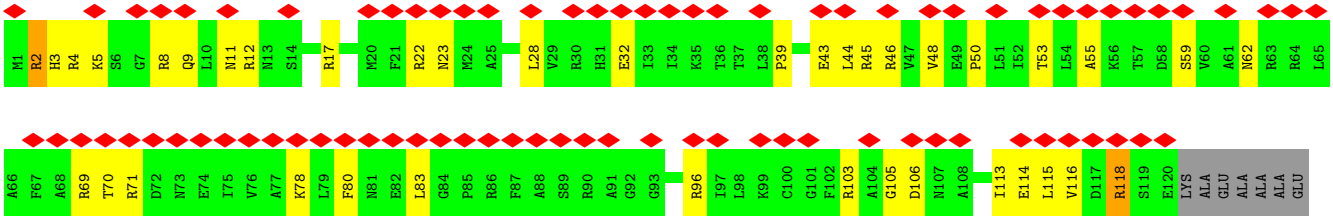
• Molecule 37: 50S ribosomal protein L15



• Molecule 38: 50S ribosomal protein L16

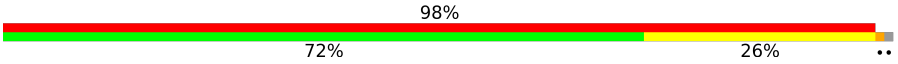


• Molecule 39: 50S ribosomal protein L17



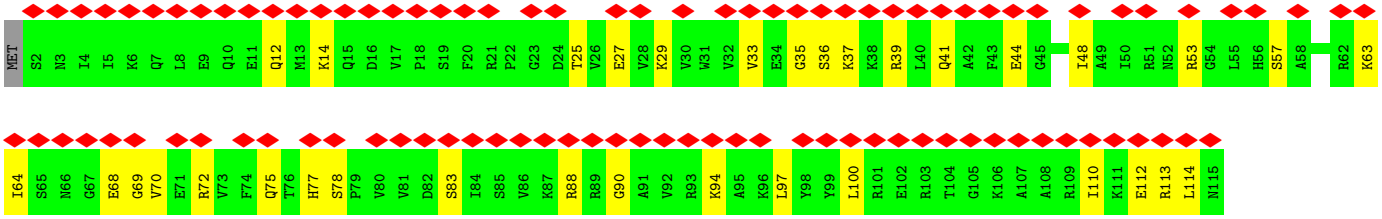
• Molecule 40: 50S ribosomal protein L18

Chain BO:



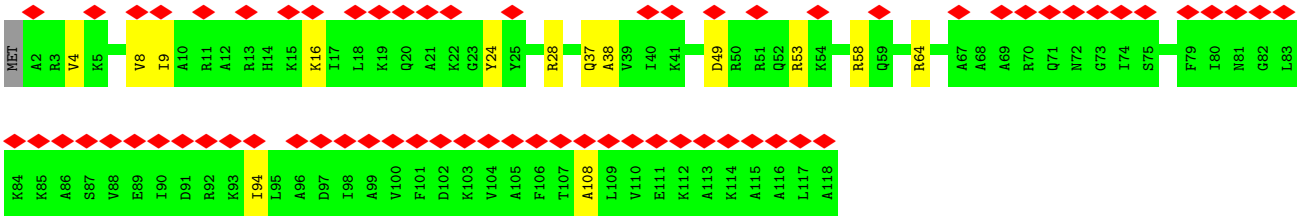
• Molecule 41: 50S ribosomal protein L19

Chain BP:



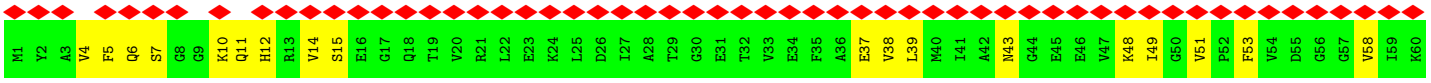
• Molecule 42: 50S ribosomal protein L20

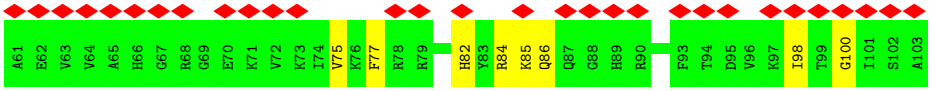
Chain BQ:



• Molecule 43: 50S ribosomal protein L21

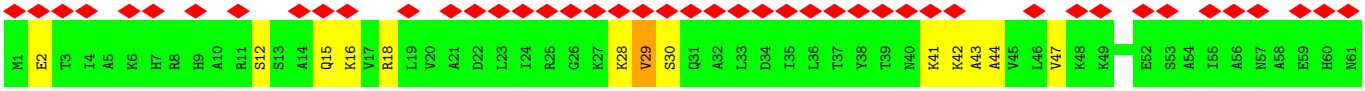
Chain BR:

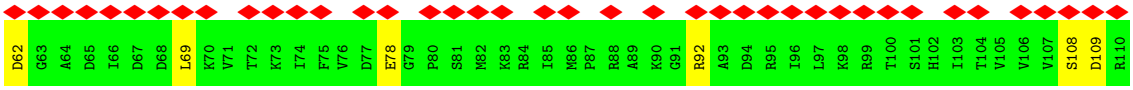




• Molecule 44: 50S ribosomal protein L22

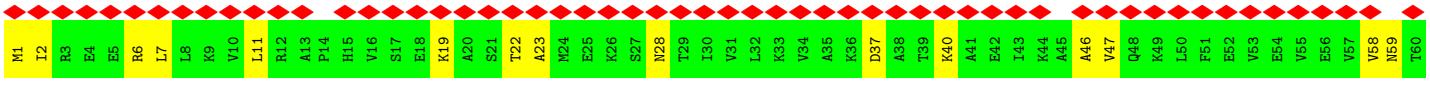
Chain BS:

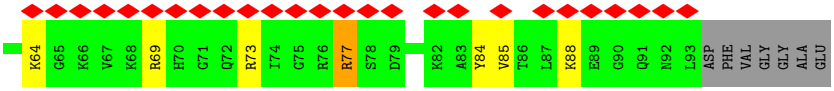




• Molecule 45: 50S ribosomal protein L23

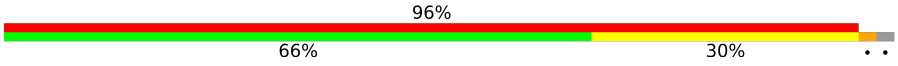
Chain BT:

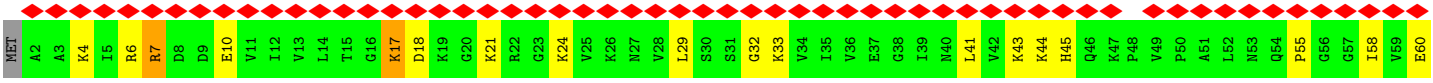


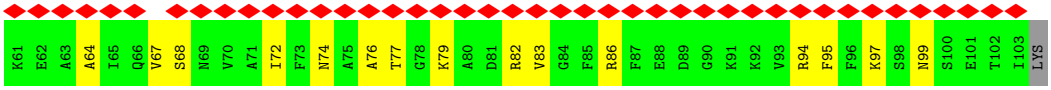


• Molecule 46: 50S ribosomal protein L24

Chain BU:

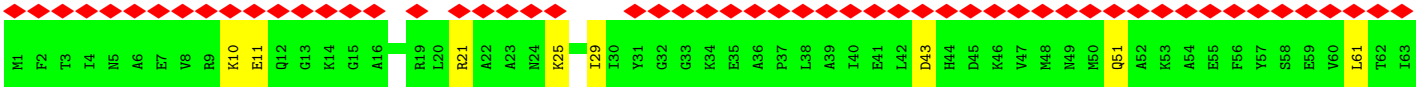


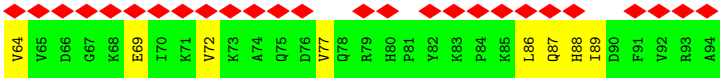




• Molecule 47: 50S ribosomal protein L25

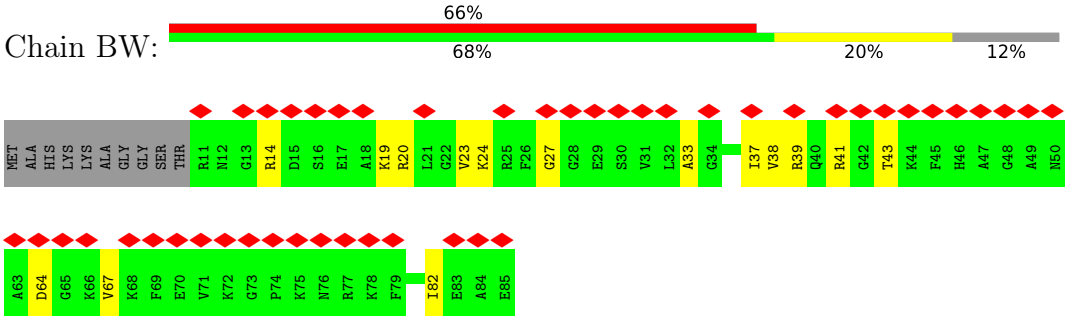
Chain BV:





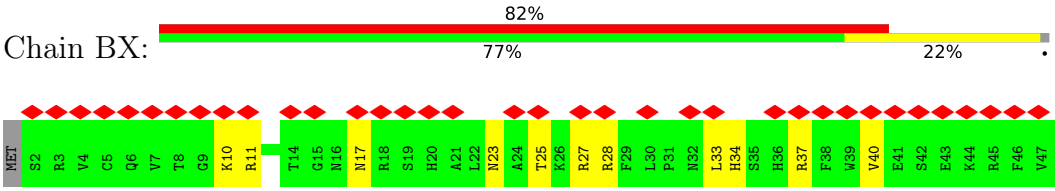
• Molecule 48: 50S ribosomal protein L27

Chain BW:



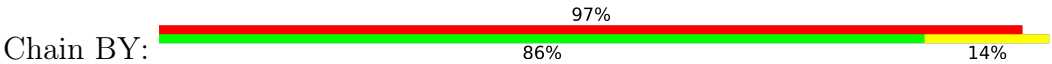
• Molecule 49: 50S ribosomal protein L28

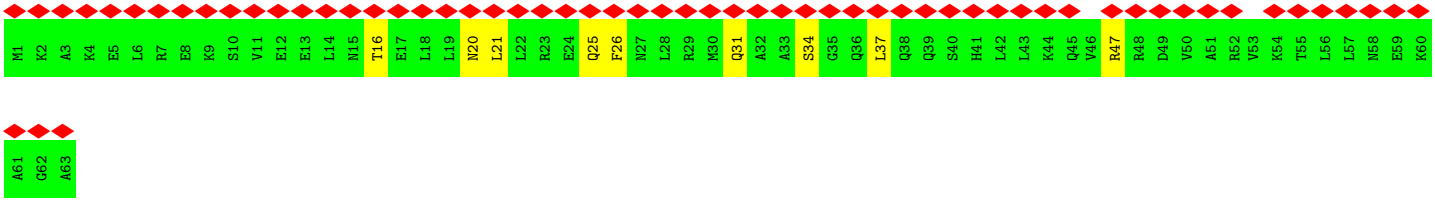
Chain BX:



• Molecule 50: 50S ribosomal protein L29

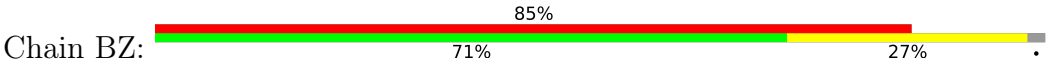
Chain BY:

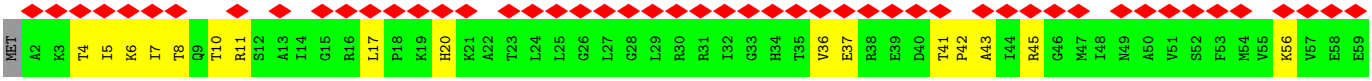




• Molecule 51: 50S ribosomal protein L30

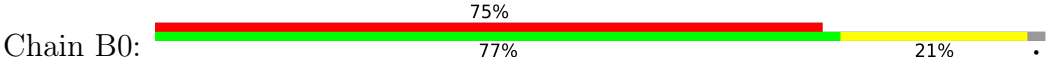
Chain BZ:

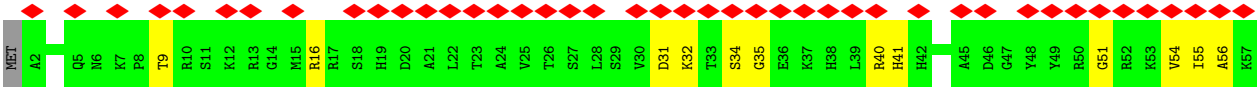




• Molecule 52: 50S ribosomal protein L32

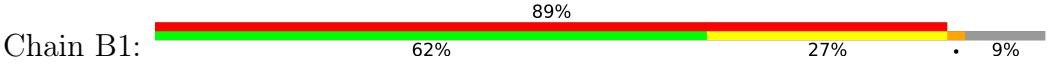
Chain B0:

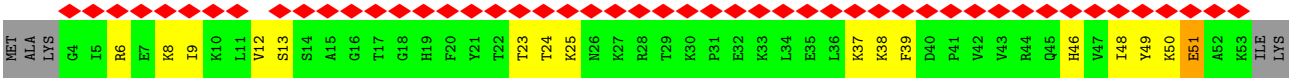




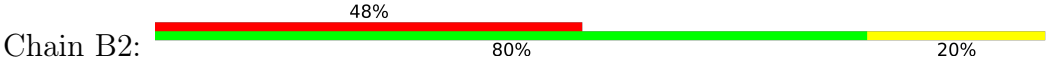
• Molecule 53: 50S ribosomal protein L33

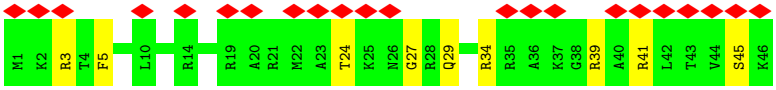
Chain B1:



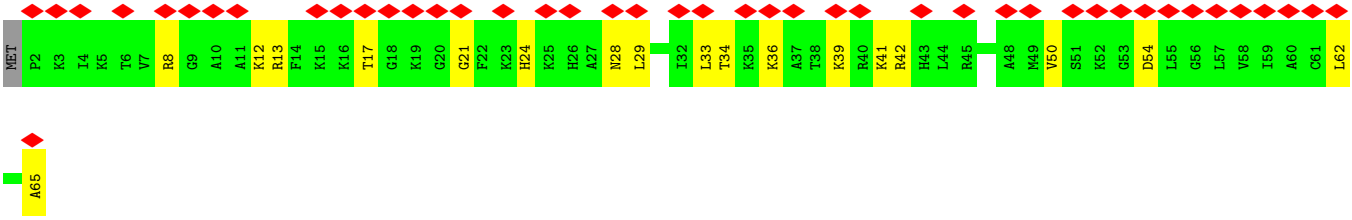


• Molecule 54: 50S ribosomal protein L34

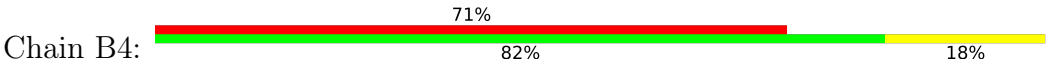


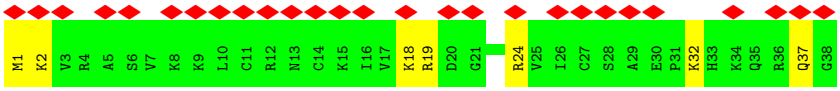


• Molecule 55: 50S ribosomal protein L35

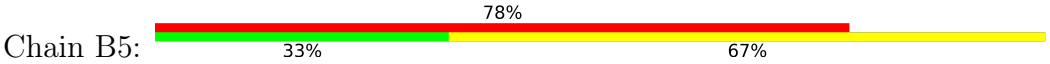


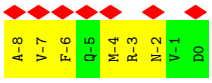
• Molecule 56: 50S ribosomal protein L36





• Molecule 57: ErmBL





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85393	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 ($e^-/Å^2$)	4	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.010	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00194	Depositor
Map size (Å)	407.74402, 407.74402, 407.74402	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 7MG, T6A, 6MZ, 3AU, ERY, 4SU, QUO, PSU, 2MA, U8U, CM0

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	2.20	1353/36965 (3.7%)	3.39	4664/57662 (8.1%)
2	AB	0.30	0/1735	0.49	0/2338
3	AC	0.25	0/1651	0.44	0/2225
4	AD	0.27	0/1665	0.47	0/2227
5	AE	0.24	0/1118	0.46	0/1504
6	AF	0.25	0/835	0.46	0/1128
7	AG	0.25	0/1195	0.42	0/1602
8	AH	0.27	0/989	0.45	0/1326
9	AI	0.28	0/1034	0.48	0/1375
10	AJ	0.31	0/796	0.53	0/1077
11	AK	0.25	0/893	0.44	0/1205
12	AL	0.25	0/969	0.45	0/1300
13	AM	0.27	0/892	0.49	0/1193
14	AN	0.24	0/785	0.42	0/1043
15	AO	0.28	0/718	0.45	0/959
16	AP	0.26	0/659	0.44	0/884
17	AQ	0.26	0/657	0.49	0/881
18	AR	0.27	0/462	0.44	0/621
19	AS	0.26	0/652	0.43	0/877
20	AT	0.25	0/671	0.43	0/888
21	AU	0.25	0/430	0.50	0/570
22	AV	3.36	21/245 (8.6%)	5.13	72/380 (18.9%)
23	AW	2.30	58/1569 (3.7%)	3.39	201/2437 (8.2%)
24	AX	2.07	48/1668 (2.9%)	2.69	139/2593 (5.4%)
25	AY	1.97	44/1554 (2.8%)	3.05	157/2416 (6.5%)
26	BA	2.25	2626/69659 (3.8%)	3.46	9154/108672 (8.4%)
27	BB	1.94	79/2828 (2.8%)	3.00	278/4410 (6.3%)
28	BC	0.25	0/2121	0.45	0/2852
29	BD	0.27	0/1586	0.45	0/2134
30	BE	0.27	0/1571	0.45	0/2113
31	BF	0.30	0/1434	0.47	0/1926
32	BG	0.27	0/1343	0.44	0/1816

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	BH	0.29	0/364	0.52	0/490
34	BI	0.28	0/1046	0.49	0/1410
35	BJ	0.27	0/1152	0.44	0/1551
36	BK	0.26	0/947	0.46	0/1268
37	BL	0.24	0/1054	0.44	0/1403
38	BM	0.26	0/1093	0.43	0/1460
39	BN	0.25	0/973	0.43	0/1301
40	BO	0.25	0/902	0.40	0/1209
41	BP	0.24	0/929	0.43	0/1242
42	BQ	0.24	0/960	0.38	0/1278
43	BR	0.25	0/829	0.43	0/1107
44	BS	0.29	0/864	0.48	0/1156
45	BT	0.23	0/744	0.43	0/994
46	BU	0.28	0/787	0.45	0/1051
47	BV	0.27	0/766	0.44	0/1025
48	BW	0.25	0/576	0.39	0/762
49	BX	0.23	0/635	0.39	0/848
50	BY	0.22	0/510	0.38	0/677
51	BZ	0.23	0/453	0.44	0/605
52	B0	0.27	0/450	0.44	0/599
53	B1	0.24	0/416	0.43	0/554
54	B2	0.20	0/380	0.37	0/498
55	B3	0.22	0/513	0.41	0/676
56	B4	0.23	0/303	0.39	0/397
57	B5	0.36	0/74	0.59	0/98
All	All	1.89	4229/159069 (2.7%)	2.97	14665/238293 (6.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
29	BD	0	1

All (4229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	20	U	C5-C6	23.31	1.55	1.34
23	AW	20	U	C5-C6	23.29	1.55	1.34
24	AX	16	U	C5-C6	23.26	1.55	1.34
24	AX	19	U	C5-C6	23.18	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	454	A	C6-N6	17.20	1.47	1.33
26	BA	1570	A	C6-N6	17.12	1.47	1.33
1	AA	74	A	C6-N6	17.11	1.47	1.33
26	BA	819	A	C6-N6	17.08	1.47	1.33
26	BA	1937	A	C6-N6	17.08	1.47	1.33
1	AA	1227	A	C6-N6	17.06	1.47	1.33
27	BB	34	A	C6-N6	17.06	1.47	1.33
1	AA	681	A	C6-N6	17.06	1.47	1.33
26	BA	479	A	C6-N6	17.05	1.47	1.33
26	BA	1641	A	C6-N6	17.05	1.47	1.33
1	AA	1005	A	C6-N6	17.04	1.47	1.33
1	AA	1374	A	C6-N6	17.04	1.47	1.33
26	BA	2513	A	C6-N6	17.04	1.47	1.33
1	AA	411	A	C6-N6	17.04	1.47	1.33
26	BA	633	A	C6-N6	17.03	1.47	1.33
26	BA	1014	A	C6-N6	17.03	1.47	1.33
1	AA	162	A	C6-N6	17.03	1.47	1.33
1	AA	431	A	C6-N6	17.02	1.47	1.33
26	BA	190	A	C6-N6	17.02	1.47	1.33
26	BA	905	A	C6-N6	17.02	1.47	1.33
26	BA	1165	A	C6-N6	17.02	1.47	1.33
26	BA	2019	A	C6-N6	17.02	1.47	1.33
26	BA	2378	A	C6-N6	17.01	1.47	1.33
1	AA	1311	A	C6-N6	17.01	1.47	1.33
26	BA	2033	A	C6-N6	17.01	1.47	1.33
1	AA	873	A	C6-N6	17.00	1.47	1.33
1	AA	1375	A	C6-N6	17.00	1.47	1.33
26	BA	2392	A	C6-N6	17.00	1.47	1.33
26	BA	556	A	C6-N6	17.00	1.47	1.33
1	AA	190	A	C6-N6	17.00	1.47	1.33
26	BA	1866	A	C6-N6	17.00	1.47	1.33
1	AA	1225	A	C6-N6	17.00	1.47	1.33
1	AA	50	A	C6-N6	16.99	1.47	1.33
1	AA	554	A	C6-N6	16.99	1.47	1.33
26	BA	52	A	C6-N6	16.99	1.47	1.33
26	BA	1469	A	C6-N6	16.99	1.47	1.33
26	BA	1241	A	C6-N6	16.99	1.47	1.33
26	BA	1590	A	C6-N6	16.99	1.47	1.33
26	BA	2154	A	C6-N6	16.98	1.47	1.33
26	BA	654	A	C6-N6	16.98	1.47	1.33
26	BA	2776	A	C6-N6	16.98	1.47	1.33
26	BA	429	A	C6-N6	16.98	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1040	A	C6-N6	16.98	1.47	1.33
26	BA	191	A	C6-N6	16.98	1.47	1.33
1	AA	155	A	C6-N6	16.98	1.47	1.33
26	BA	1194	A	C6-N6	16.98	1.47	1.33
26	BA	2418	A	C6-N6	16.98	1.47	1.33
1	AA	393	A	C6-N6	16.98	1.47	1.33
1	AA	977	A	C6-N6	16.98	1.47	1.33
26	BA	127	A	C6-N6	16.97	1.47	1.33
1	AA	547	A	C6-N6	16.97	1.47	1.33
1	AA	1000	A	C6-N6	16.97	1.47	1.33
26	BA	2176	A	C6-N6	16.97	1.47	1.33
1	AA	228	A	C6-N6	16.97	1.47	1.33
1	AA	456	A	C6-N6	16.97	1.47	1.33
26	BA	2430	A	C6-N6	16.97	1.47	1.33
1	AA	649	A	C6-N6	16.97	1.47	1.33
1	AA	907	A	C6-N6	16.97	1.47	1.33
1	AA	1410	A	C6-N6	16.97	1.47	1.33
26	BA	42	A	C6-N6	16.97	1.47	1.33
26	BA	1284	A	C6-N6	16.97	1.47	1.33
1	AA	572	A	C6-N6	16.96	1.47	1.33
1	AA	908	A	C6-N6	16.96	1.47	1.33
1	AA	1248	A	C6-N6	16.96	1.47	1.33
26	BA	1969	A	C6-N6	16.96	1.47	1.33
26	BA	2589	A	C6-N6	16.96	1.47	1.33
1	AA	1437	A	C6-N6	16.96	1.47	1.33
1	AA	414	A	C6-N6	16.96	1.47	1.33
1	AA	1513	A	C6-N6	16.96	1.47	1.33
26	BA	1508	A	C6-N6	16.96	1.47	1.33
1	AA	1441	A	C6-N6	16.96	1.47	1.33
1	AA	1500	A	C6-N6	16.96	1.47	1.33
26	BA	2297	A	C6-N6	16.96	1.47	1.33
1	AA	1146	A	C6-N6	16.95	1.47	1.33
1	AA	1261	A	C6-N6	16.95	1.47	1.33
26	BA	749	A	C6-N6	16.95	1.47	1.33
1	AA	243	A	C6-N6	16.95	1.47	1.33
26	BA	38	A	C6-N6	16.95	1.47	1.33
26	BA	668	A	C6-N6	16.95	1.47	1.33
26	BA	1246	A	C6-N6	16.95	1.47	1.33
26	BA	1490	A	C6-N6	16.95	1.47	1.33
26	BA	2665	A	C6-N6	16.95	1.47	1.33
26	BA	792	A	C6-N6	16.95	1.47	1.33
26	BA	2266	A	C6-N6	16.95	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2366	A	C6-N6	16.95	1.47	1.33
1	AA	609	A	C6-N6	16.95	1.47	1.33
1	AA	790	A	C6-N6	16.95	1.47	1.33
1	AA	901	A	C6-N6	16.95	1.47	1.33
1	AA	1418	A	C6-N6	16.95	1.47	1.33
26	BA	352	A	C6-N6	16.95	1.47	1.33
26	BA	1981	A	C6-N6	16.95	1.47	1.33
26	BA	2632	A	C6-N6	16.95	1.47	1.33
26	BA	1987	A	C6-N6	16.95	1.47	1.33
26	BA	2781	A	C6-N6	16.95	1.47	1.33
1	AA	1319	A	C6-N6	16.95	1.47	1.33
26	BA	401	A	C6-N6	16.95	1.47	1.33
26	BA	447	A	C6-N6	16.95	1.47	1.33
26	BA	2821	A	C6-N6	16.95	1.47	1.33
1	AA	860	A	C6-N6	16.95	1.47	1.33
1	AA	1329	A	C6-N6	16.95	1.47	1.33
26	BA	1054	A	C6-N6	16.95	1.47	1.33
26	BA	1336	A	C6-N6	16.95	1.47	1.33
1	AA	59	A	C6-N6	16.94	1.47	1.33
26	BA	432	A	C6-N6	16.94	1.47	1.33
26	BA	960	A	C6-N6	16.94	1.47	1.33
26	BA	2602	A	C6-N6	16.94	1.47	1.33
26	BA	2748	A	C6-N6	16.94	1.47	1.33
1	AA	1014	A	C6-N6	16.94	1.47	1.33
1	AA	1110	A	C6-N6	16.94	1.47	1.33
26	BA	614	A	C6-N6	16.94	1.47	1.33
26	BA	1366	A	C6-N6	16.94	1.47	1.33
1	AA	983	A	C6-N6	16.94	1.47	1.33
26	BA	340	A	C6-N6	16.94	1.47	1.33
26	BA	945	A	C6-N6	16.94	1.47	1.33
26	BA	2205	A	C6-N6	16.94	1.47	1.33
1	AA	825	A	C6-N6	16.94	1.47	1.33
1	AA	1179	A	C6-N6	16.94	1.47	1.33
26	BA	310	A	C6-N6	16.94	1.47	1.33
26	BA	1757	A	C6-N6	16.94	1.47	1.33
26	BA	2340	A	C6-N6	16.94	1.47	1.33
26	BA	2435	A	C6-N6	16.94	1.47	1.33
1	AA	309	A	C6-N6	16.94	1.47	1.33
1	AA	1483	A	C6-N6	16.94	1.47	1.33
26	BA	439	A	C6-N6	16.94	1.47	1.33
26	BA	984	A	C6-N6	16.94	1.47	1.33
26	BA	1304	A	C6-N6	16.94	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2426	A	C6-N6	16.94	1.47	1.33
26	BA	2468	A	C6-N6	16.94	1.47	1.33
1	AA	749	A	C6-N6	16.94	1.47	1.33
1	AA	77	A	C6-N6	16.93	1.47	1.33
26	BA	203	A	C6-N6	16.93	1.47	1.33
26	BA	2434	A	C6-N6	16.93	1.47	1.33
26	BA	2736	A	C6-N6	16.93	1.47	1.33
26	BA	2893	A	C6-N6	16.93	1.47	1.33
26	BA	1151	A	C6-N6	16.93	1.47	1.33
26	BA	2273	A	C6-N6	16.93	1.47	1.33
26	BA	1205	A	C6-N6	16.93	1.47	1.33
26	BA	1274	A	C6-N6	16.93	1.47	1.33
26	BA	2042	A	C6-N6	16.93	1.47	1.33
1	AA	60	A	C6-N6	16.93	1.47	1.33
26	BA	1070	A	C6-N6	16.93	1.47	1.33
26	BA	1384	A	C6-N6	16.93	1.47	1.33
26	BA	2823	A	C6-N6	16.93	1.47	1.33
1	AA	994	A	C6-N6	16.93	1.47	1.33
1	AA	1280	A	C6-N6	16.93	1.47	1.33
26	BA	126	A	C6-N6	16.93	1.47	1.33
26	BA	309	A	C6-N6	16.93	1.47	1.33
26	BA	513	A	C6-N6	16.93	1.47	1.33
26	BA	2530	A	C6-N6	16.93	1.47	1.33
1	AA	900	A	C6-N6	16.93	1.47	1.33
27	BB	101	A	C6-N6	16.93	1.47	1.33
1	AA	415	A	C6-N6	16.93	1.47	1.33
1	AA	687	A	C6-N6	16.93	1.47	1.33
23	AW	42	A	C6-N6	16.93	1.47	1.33
26	BA	181	A	C6-N6	16.93	1.47	1.33
26	BA	2705	A	C6-N6	16.93	1.47	1.33
26	BA	2899	A	C6-N6	16.93	1.47	1.33
26	BA	219	A	C6-N6	16.92	1.47	1.33
1	AA	131	A	C6-N6	16.92	1.47	1.33
1	AA	1274	A	C6-N6	16.92	1.47	1.33
1	AA	1468	A	C6-N6	16.92	1.47	1.33
26	BA	2860	A	C6-N6	16.92	1.47	1.33
1	AA	179	A	C6-N6	16.92	1.47	1.33
23	AW	59	A	C6-N6	16.92	1.47	1.33
26	BA	1890	A	C6-N6	16.92	1.47	1.33
26	BA	1998	A	C6-N6	16.92	1.47	1.33
26	BA	2071	A	C6-N6	16.92	1.47	1.33
26	BA	2227	A	C6-N6	16.92	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2670	A	C6-N6	16.92	1.47	1.33
26	BA	422	A	C6-N6	16.92	1.47	1.33
26	BA	1571	A	C6-N6	16.92	1.47	1.33
26	BA	1749	A	C6-N6	16.92	1.47	1.33
1	AA	253	A	C6-N6	16.92	1.47	1.33
1	AA	498	A	C6-N6	16.92	1.47	1.33
23	AW	41	A	C6-N6	16.92	1.47	1.33
25	AY	26	A	C6-N6	16.92	1.47	1.33
26	BA	718	A	C6-N6	16.92	1.47	1.33
26	BA	1021	A	C6-N6	16.92	1.47	1.33
26	BA	1385	A	C6-N6	16.92	1.47	1.33
26	BA	1711	A	C6-N6	16.92	1.47	1.33
1	AA	7	A	C6-N6	16.92	1.47	1.33
1	AA	167	A	C6-N6	16.92	1.47	1.33
26	BA	2814	A	C6-N6	16.92	1.47	1.33
1	AA	958	A	C6-N6	16.91	1.47	1.33
1	AA	978	A	C6-N6	16.91	1.47	1.33
26	BA	402	A	C6-N6	16.91	1.47	1.33
26	BA	1593	A	C6-N6	16.91	1.47	1.33
26	BA	1970	A	C6-N6	16.91	1.47	1.33
26	BA	2309	A	C6-N6	16.91	1.47	1.33
26	BA	2381	A	C6-N6	16.91	1.47	1.33
26	BA	2679	A	C6-N6	16.91	1.47	1.33
1	AA	648	A	C6-N6	16.91	1.47	1.33
26	BA	195	A	C6-N6	16.91	1.47	1.33
26	BA	1393	A	C6-N6	16.91	1.47	1.33
26	BA	1780	A	C6-N6	16.91	1.47	1.33
1	AA	363	A	C6-N6	16.91	1.47	1.33
1	AA	787	A	C6-N6	16.91	1.47	1.33
1	AA	1036	A	C6-N6	16.91	1.47	1.33
1	AA	1502	A	C6-N6	16.91	1.47	1.33
1	AA	1531	A	C6-N6	16.91	1.47	1.33
26	BA	751	A	C6-N6	16.91	1.47	1.33
26	BA	2009	A	C6-N6	16.91	1.47	1.33
26	BA	2030	A	C6-N6	16.91	1.47	1.33
26	BA	2117	A	C6-N6	16.91	1.47	1.33
26	BA	2634	A	C6-N6	16.91	1.47	1.33
26	BA	2662	A	C6-N6	16.91	1.47	1.33
1	AA	101	A	C6-N6	16.91	1.47	1.33
1	AA	1306	A	C6-N6	16.91	1.47	1.33
26	BA	2082	A	C6-N6	16.91	1.47	1.33
26	BA	2778	A	C6-N6	16.91	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BB	29	A	C6-N6	16.91	1.47	1.33
1	AA	441	A	C6-N6	16.91	1.47	1.33
1	AA	676	A	C6-N6	16.91	1.47	1.33
1	AA	702	A	C6-N6	16.91	1.47	1.33
1	AA	747	A	C6-N6	16.91	1.47	1.33
1	AA	816	A	C6-N6	16.91	1.47	1.33
1	AA	959	A	C6-N6	16.91	1.47	1.33
1	AA	1080	A	C6-N6	16.91	1.47	1.33
26	BA	480	A	C6-N6	16.91	1.47	1.33
26	BA	631	A	C6-N6	16.91	1.47	1.33
26	BA	727	A	C6-N6	16.91	1.47	1.33
26	BA	1373	A	C6-N6	16.91	1.47	1.33
26	BA	1580	A	C6-N6	16.91	1.47	1.33
26	BA	1938	A	C6-N6	16.91	1.47	1.33
26	BA	1960	A	C6-N6	16.91	1.47	1.33
26	BA	2142	A	C6-N6	16.91	1.47	1.33
26	BA	2587	A	C6-N6	16.91	1.47	1.33
26	BA	2590	A	C6-N6	16.91	1.47	1.33
27	BB	15	A	C6-N6	16.91	1.47	1.33
1	AA	51	A	C6-N6	16.91	1.47	1.33
1	AA	640	A	C6-N6	16.91	1.47	1.33
26	BA	14	A	C6-N6	16.91	1.47	1.33
26	BA	347	A	C6-N6	16.91	1.47	1.33
26	BA	1395	A	C6-N6	16.91	1.47	1.33
26	BA	1505	A	C6-N6	16.91	1.47	1.33
1	AA	196	A	C6-N6	16.91	1.47	1.33
1	AA	780	A	C6-N6	16.91	1.47	1.33
23	AW	66	A	C6-N6	16.91	1.47	1.33
24	AX	14	A	C6-N6	16.91	1.47	1.33
26	BA	111	A	C6-N6	16.91	1.47	1.33
26	BA	892	A	C6-N6	16.91	1.47	1.33
26	BA	943	A	C6-N6	16.91	1.47	1.33
26	BA	1029	A	C6-N6	16.91	1.47	1.33
26	BA	1144	A	C6-N6	16.91	1.47	1.33
26	BA	1237	A	C6-N6	16.91	1.47	1.33
26	BA	1403	A	C6-N6	16.91	1.47	1.33
1	AA	19	A	C6-N6	16.90	1.47	1.33
1	AA	468	A	C6-N6	16.90	1.47	1.33
26	BA	156	A	C6-N6	16.90	1.47	1.33
26	BA	507	A	C6-N6	16.90	1.47	1.33
26	BA	699	A	C6-N6	16.90	1.47	1.33
26	BA	849	A	C6-N6	16.90	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1077	A	C6-N6	16.90	1.47	1.33
26	BA	1453	A	C6-N6	16.90	1.47	1.33
26	BA	2887	A	C6-N6	16.90	1.47	1.33
1	AA	510	A	C6-N6	16.90	1.47	1.33
1	AA	815	A	C6-N6	16.90	1.47	1.33
1	AA	819	A	C6-N6	16.90	1.47	1.33
1	AA	1408	A	C6-N6	16.90	1.47	1.33
25	AY	69	A	C6-N6	16.90	1.47	1.33
26	BA	213	A	C6-N6	16.90	1.47	1.33
26	BA	979	A	C6-N6	16.90	1.47	1.33
26	BA	1086	A	C6-N6	16.90	1.47	1.33
26	BA	1871	A	C6-N6	16.90	1.47	1.33
26	BA	2198	A	C6-N6	16.90	1.47	1.33
1	AA	704	A	C6-N6	16.90	1.47	1.33
26	BA	1302	A	C6-N6	16.90	1.47	1.33
26	BA	1744	A	C6-N6	16.90	1.47	1.33
26	BA	1746	A	C6-N6	16.90	1.47	1.33
26	BA	2270	A	C6-N6	16.90	1.47	1.33
1	AA	44	A	C6-N6	16.90	1.47	1.33
1	AA	72	A	C6-N6	16.90	1.47	1.33
1	AA	181	A	C6-N6	16.90	1.47	1.33
1	AA	743	A	C6-N6	16.90	1.47	1.33
23	AW	26	A	C6-N6	16.90	1.47	1.33
23	AW	58	A	C6-N6	16.90	1.47	1.33
26	BA	1073	A	C6-N6	16.90	1.47	1.33
26	BA	1126	A	C6-N6	16.90	1.47	1.33
26	BA	2114	A	C6-N6	16.90	1.47	1.33
26	BA	2322	A	C6-N6	16.90	1.47	1.33
26	BA	2482	A	C6-N6	16.90	1.47	1.33
1	AA	349	A	C6-N6	16.90	1.47	1.33
1	AA	559	A	C6-N6	16.90	1.47	1.33
1	AA	935	A	C6-N6	16.90	1.47	1.33
1	AA	1433	A	C6-N6	16.90	1.47	1.33
26	BA	742	A	C6-N6	16.90	1.47	1.33
1	AA	66	A	C6-N6	16.90	1.47	1.33
1	AA	831	A	C6-N6	16.90	1.47	1.33
1	AA	1534	A	C6-N6	16.90	1.47	1.33
23	AW	69	A	C6-N6	16.90	1.47	1.33
26	BA	83	A	C6-N6	16.90	1.47	1.33
26	BA	160	A	C6-N6	16.90	1.47	1.33
26	BA	165	A	C6-N6	16.90	1.47	1.33
26	BA	471	A	C6-N6	16.90	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	632	A	C6-N6	16.90	1.47	1.33
26	BA	844	A	C6-N6	16.90	1.47	1.33
26	BA	972	A	C6-N6	16.90	1.47	1.33
26	BA	1596	A	C6-N6	16.90	1.47	1.33
26	BA	2352	A	C6-N6	16.90	1.47	1.33
1	AA	1176	A	C6-N6	16.89	1.47	1.33
26	BA	1918	A	C6-N6	16.89	1.47	1.33
1	AA	250	A	C6-N6	16.89	1.47	1.33
1	AA	300	A	C6-N6	16.89	1.47	1.33
1	AA	496	A	C6-N6	16.89	1.47	1.33
1	AA	1019	A	C6-N6	16.89	1.47	1.33
22	AV	17	A	C6-N6	16.89	1.47	1.33
26	BA	505	A	C6-N6	16.89	1.47	1.33
26	BA	899	A	C6-N6	16.89	1.47	1.33
26	BA	1597	A	C6-N6	16.89	1.47	1.33
26	BA	1630	A	C6-N6	16.89	1.47	1.33
26	BA	1952	A	C6-N6	16.89	1.47	1.33
26	BA	2284	A	C6-N6	16.89	1.47	1.33
26	BA	2439	A	C6-N6	16.89	1.47	1.33
26	BA	693	A	C6-N6	16.89	1.47	1.33
26	BA	1413	A	C6-N6	16.89	1.47	1.33
26	BA	1495	A	C6-N6	16.89	1.47	1.33
26	BA	2183	A	C6-N6	16.89	1.47	1.33
1	AA	116	A	C6-N6	16.89	1.47	1.33
1	AA	373	A	C6-N6	16.89	1.47	1.33
1	AA	1150	A	C6-N6	16.89	1.47	1.33
26	BA	63	A	C6-N6	16.89	1.47	1.33
26	BA	64	A	C6-N6	16.89	1.47	1.33
26	BA	89	A	C6-N6	16.89	1.47	1.33
26	BA	103	A	C6-N6	16.89	1.47	1.33
26	BA	590	A	C6-N6	16.89	1.47	1.33
26	BA	603	A	C6-N6	16.89	1.47	1.33
26	BA	1262	A	C6-N6	16.89	1.47	1.33
26	BA	1367	A	C6-N6	16.89	1.47	1.33
26	BA	1701	A	C6-N6	16.89	1.47	1.33
26	BA	1953	A	C6-N6	16.89	1.47	1.33
26	BA	1966	A	C6-N6	16.89	1.47	1.33
26	BA	2753	A	C6-N6	16.89	1.47	1.33
26	BA	2761	A	C6-N6	16.89	1.47	1.33
1	AA	1111	A	C6-N6	16.89	1.47	1.33
1	AA	1271	A	C6-N6	16.89	1.47	1.33
1	AA	1346	A	C6-N6	16.89	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1398	A	C6-N6	16.89	1.47	1.33
22	AV	22	A	C6-N6	16.89	1.47	1.33
23	AW	73	A	C6-N6	16.89	1.47	1.33
25	AY	58	A	C6-N6	16.89	1.47	1.33
26	BA	118	A	C6-N6	16.89	1.47	1.33
26	BA	959	A	C6-N6	16.89	1.47	1.33
26	BA	1095	A	C6-N6	16.89	1.47	1.33
26	BA	1433	A	C6-N6	16.89	1.47	1.33
26	BA	1583	A	C6-N6	16.89	1.47	1.33
26	BA	2058	A	C6-N6	16.89	1.47	1.33
27	BB	57	A	C6-N6	16.89	1.47	1.33
1	AA	466	A	C6-N6	16.89	1.47	1.33
1	AA	487	A	C6-N6	16.89	1.47	1.33
1	AA	1287	A	C6-N6	16.89	1.47	1.33
24	AX	21	A	C6-N6	16.89	1.47	1.33
26	BA	49	A	C6-N6	16.89	1.47	1.33
26	BA	74	A	C6-N6	16.89	1.47	1.33
26	BA	477	A	C6-N6	16.89	1.47	1.33
26	BA	1503	A	C6-N6	16.89	1.47	1.33
26	BA	2314	A	C6-N6	16.89	1.47	1.33
1	AA	2	A	C6-N6	16.89	1.47	1.33
1	AA	152	A	C6-N6	16.89	1.47	1.33
1	AA	315	A	C6-N6	16.89	1.47	1.33
1	AA	338	A	C6-N6	16.89	1.47	1.33
1	AA	1004	A	C6-N6	16.89	1.47	1.33
1	AA	1480	A	C6-N6	16.89	1.47	1.33
26	BA	28	A	C6-N6	16.89	1.47	1.33
26	BA	609	A	C6-N6	16.89	1.47	1.33
26	BA	734	A	C6-N6	16.89	1.47	1.33
26	BA	764	A	C6-N6	16.89	1.47	1.33
26	BA	947	A	C6-N6	16.89	1.47	1.33
26	BA	980	A	C6-N6	16.89	1.47	1.33
26	BA	1285	A	C6-N6	16.89	1.47	1.33
26	BA	1679	A	C6-N6	16.89	1.47	1.33
26	BA	1927	A	C6-N6	16.89	1.47	1.33
27	BB	73	A	C6-N6	16.89	1.47	1.33
1	AA	1339	A	C6-N6	16.88	1.47	1.33
26	BA	478	A	C6-N6	16.88	1.47	1.33
26	BA	1147	A	C6-N6	16.88	1.47	1.33
26	BA	1365	A	C6-N6	16.88	1.47	1.33
26	BA	1928	A	C6-N6	16.88	1.47	1.33
26	BA	2750	A	C6-N6	16.88	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2829	A	C6-N6	16.88	1.47	1.33
1	AA	80	A	C6-N6	16.88	1.47	1.33
1	AA	129	A	C6-N6	16.88	1.47	1.33
1	AA	263	A	C6-N6	16.88	1.47	1.33
1	AA	563	A	C6-N6	16.88	1.47	1.33
1	AA	845	A	C6-N6	16.88	1.47	1.33
1	AA	1204	A	C6-N6	16.88	1.47	1.33
1	AA	1507	A	C6-N6	16.88	1.47	1.33
26	BA	104	A	C6-N6	16.88	1.47	1.33
26	BA	282	A	C6-N6	16.88	1.47	1.33
26	BA	497	A	C6-N6	16.88	1.47	1.33
26	BA	829	A	C6-N6	16.88	1.47	1.33
26	BA	1080	A	C6-N6	16.88	1.47	1.33
26	BA	1175	A	C6-N6	16.88	1.47	1.33
26	BA	1772	A	C6-N6	16.88	1.47	1.33
26	BA	2003	A	C6-N6	16.88	1.47	1.33
26	BA	2013	A	C6-N6	16.88	1.47	1.33
26	BA	2792	A	C6-N6	16.88	1.47	1.33
26	BA	2809	A	C6-N6	16.88	1.47	1.33
1	AA	448	A	C6-N6	16.88	1.47	1.33
26	BA	322	A	C6-N6	16.88	1.47	1.33
26	BA	344	A	C6-N6	16.88	1.47	1.33
26	BA	781	A	C6-N6	16.88	1.47	1.33
26	BA	1913	A	C6-N6	16.88	1.47	1.33
26	BA	2837	A	C6-N6	16.88	1.47	1.33
1	AA	223	A	C6-N6	16.88	1.47	1.33
1	AA	246	A	C6-N6	16.88	1.47	1.33
1	AA	607	A	C6-N6	16.88	1.47	1.33
1	AA	892	A	C6-N6	16.88	1.47	1.33
1	AA	1413	A	C6-N6	16.88	1.47	1.33
26	BA	91	A	C6-N6	16.88	1.47	1.33
26	BA	1134	A	C6-N6	16.88	1.47	1.33
26	BA	1322	A	C6-N6	16.88	1.47	1.33
26	BA	1535	A	C6-N6	16.88	1.47	1.33
26	BA	2171	A	C6-N6	16.88	1.47	1.33
26	BA	2564	A	C6-N6	16.88	1.47	1.33
26	BA	2654	A	C6-N6	16.88	1.47	1.33
26	BA	2851	A	C6-N6	16.88	1.47	1.33
1	AA	313	A	C6-N6	16.88	1.47	1.33
1	AA	532	A	C6-N6	16.88	1.47	1.33
23	AW	51	A	C6-N6	16.88	1.47	1.33
26	BA	125	A	C6-N6	16.88	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	155	A	C6-N6	16.88	1.47	1.33
26	BA	1008	A	C6-N6	16.88	1.47	1.33
26	BA	1204	A	C6-N6	16.88	1.47	1.33
26	BA	1213	A	C6-N6	16.88	1.47	1.33
26	BA	1551	A	C6-N6	16.88	1.47	1.33
26	BA	2281	A	C6-N6	16.88	1.47	1.33
26	BA	2476	A	C6-N6	16.88	1.47	1.33
26	BA	2721	A	C6-N6	16.88	1.47	1.33
26	BA	2872	A	C6-N6	16.88	1.47	1.33
1	AA	560	A	C6-N6	16.88	1.47	1.33
1	AA	715	A	C6-N6	16.88	1.47	1.33
1	AA	1188	A	C6-N6	16.88	1.47	1.33
1	AA	1256	A	C6-N6	16.88	1.47	1.33
1	AA	1428	A	C6-N6	16.88	1.47	1.33
25	AY	35	A	C6-N6	16.88	1.47	1.33
26	BA	199	A	C6-N6	16.88	1.47	1.33
26	BA	368	A	C6-N6	16.88	1.47	1.33
26	BA	453	A	C6-N6	16.88	1.47	1.33
26	BA	627	A	C6-N6	16.88	1.47	1.33
26	BA	917	A	C6-N6	16.88	1.47	1.33
26	BA	1553	A	C6-N6	16.88	1.47	1.33
26	BA	1810	A	C6-N6	16.88	1.47	1.33
26	BA	2031	A	C6-N6	16.88	1.47	1.33
26	BA	2311	A	C6-N6	16.88	1.47	1.33
1	AA	282	A	C6-N6	16.88	1.47	1.33
26	BA	173	A	C6-N6	16.88	1.47	1.33
26	BA	342	A	C6-N6	16.88	1.47	1.33
26	BA	753	A	C6-N6	16.88	1.47	1.33
26	BA	2453	A	C6-N6	16.88	1.47	1.33
1	AA	71	A	C6-N6	16.87	1.47	1.33
1	AA	78	A	C6-N6	16.87	1.47	1.33
1	AA	767	A	C6-N6	16.87	1.47	1.33
25	AY	66	A	C6-N6	16.87	1.47	1.33
26	BA	19	A	C6-N6	16.87	1.47	1.33
26	BA	1010	A	C6-N6	16.87	1.47	1.33
26	BA	2135	A	C6-N6	16.87	1.47	1.33
26	BA	2274	A	C6-N6	16.87	1.47	1.33
26	BA	2407	A	C6-N6	16.87	1.47	1.33
26	BA	2758	A	C6-N6	16.87	1.47	1.33
27	BB	46	A	C6-N6	16.87	1.47	1.33
1	AA	1016	A	C6-N6	16.87	1.47	1.33
1	AA	1257	A	C6-N6	16.87	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	430	A	C6-N6	16.87	1.47	1.33
26	BA	1133	A	C6-N6	16.87	1.47	1.33
26	BA	1286	A	C6-N6	16.87	1.47	1.33
26	BA	1872	A	C6-N6	16.87	1.47	1.33
1	AA	694	A	C6-N6	16.87	1.47	1.33
1	AA	1169	A	C6-N6	16.87	1.47	1.33
1	AA	1396	A	C6-N6	16.87	1.47	1.33
1	AA	1519	A	C6-N6	16.87	1.47	1.33
22	AV	20	A	C6-N6	16.87	1.47	1.33
23	AW	76	A	C6-N6	16.87	1.47	1.33
26	BA	217	A	C6-N6	16.87	1.47	1.33
26	BA	231	A	C6-N6	16.87	1.47	1.33
26	BA	345	A	C6-N6	16.87	1.47	1.33
26	BA	528	A	C6-N6	16.87	1.47	1.33
26	BA	833	A	C6-N6	16.87	1.47	1.33
26	BA	1027	A	C6-N6	16.87	1.47	1.33
26	BA	1039	A	C6-N6	16.87	1.47	1.33
26	BA	1129	A	C6-N6	16.87	1.47	1.33
26	BA	1672	A	C6-N6	16.87	1.47	1.33
26	BA	1858	A	C6-N6	16.87	1.47	1.33
26	BA	1932	A	C6-N6	16.87	1.47	1.33
26	BA	2014	A	C6-N6	16.87	1.47	1.33
26	BA	2850	A	C6-N6	16.87	1.47	1.33
1	AA	16	A	C6-N6	16.87	1.47	1.33
1	AA	197	A	C6-N6	16.87	1.47	1.33
1	AA	366	A	C6-N6	16.87	1.47	1.33
1	AA	675	A	C6-N6	16.87	1.47	1.33
1	AA	913	A	C6-N6	16.87	1.47	1.33
1	AA	1130	A	C6-N6	16.87	1.47	1.33
1	AA	1318	A	C6-N6	16.87	1.47	1.33
25	AY	41	A	C6-N6	16.87	1.47	1.33
26	BA	354	A	C6-N6	16.87	1.47	1.33
26	BA	482	A	C6-N6	16.87	1.47	1.33
26	BA	666	A	C6-N6	16.87	1.47	1.33
26	BA	1169	A	C6-N6	16.87	1.47	1.33
26	BA	1754	A	C6-N6	16.87	1.47	1.33
26	BA	1755	A	C6-N6	16.87	1.47	1.33
26	BA	2191	A	C6-N6	16.87	1.47	1.33
26	BA	2317	A	C6-N6	16.87	1.47	1.33
27	BB	104	A	C6-N6	16.87	1.47	1.33
1	AA	574	A	C6-N6	16.87	1.47	1.33
1	AA	1093	A	C6-N6	16.87	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1101	A	C6-N6	16.87	1.47	1.33
1	AA	1368	A	C6-N6	16.87	1.47	1.33
26	BA	272	A	C6-N6	16.87	1.47	1.33
26	BA	1847	A	C6-N6	16.87	1.47	1.33
26	BA	2090	A	C6-N6	16.87	1.47	1.33
26	BA	2635	A	C6-N6	16.87	1.47	1.33
1	AA	320	A	C6-N6	16.86	1.47	1.33
1	AA	781	A	C6-N6	16.86	1.47	1.33
1	AA	1042	A	C6-N6	16.86	1.47	1.33
1	AA	1499	A	C6-N6	16.86	1.47	1.33
26	BA	176	A	C6-N6	16.86	1.47	1.33
26	BA	299	A	C6-N6	16.86	1.47	1.33
26	BA	470	A	C6-N6	16.86	1.47	1.33
26	BA	504	A	C6-N6	16.86	1.47	1.33
26	BA	1069	A	C6-N6	16.86	1.47	1.33
26	BA	1652	A	C6-N6	16.86	1.47	1.33
26	BA	2051	A	C6-N6	16.86	1.47	1.33
26	BA	2097	A	C6-N6	16.86	1.47	1.33
26	BA	2108	A	C6-N6	16.86	1.47	1.33
26	BA	2813	A	C6-N6	16.86	1.47	1.33
1	AA	1092	A	C6-N6	16.86	1.47	1.33
1	AA	1197	A	C6-N6	16.86	1.47	1.33
1	AA	1246	A	C6-N6	16.86	1.47	1.33
1	AA	1360	A	C6-N6	16.86	1.47	1.33
25	AY	73	A	C6-N6	16.86	1.47	1.33
26	BA	196	A	C6-N6	16.86	1.47	1.33
26	BA	1700	A	C6-N6	16.86	1.47	1.33
26	BA	1785	A	C6-N6	16.86	1.47	1.33
26	BA	1912	A	C6-N6	16.86	1.47	1.33
26	BA	2062	A	C6-N6	16.86	1.47	1.33
26	BA	2101	A	C6-N6	16.86	1.47	1.33
1	AA	192	A	C6-N6	16.86	1.47	1.33
1	AA	329	A	C6-N6	16.86	1.47	1.33
24	AX	26	A	C6-N6	16.86	1.47	1.33
26	BA	101	A	C6-N6	16.86	1.47	1.33
26	BA	1090	A	C6-N6	16.86	1.47	1.33
26	BA	1103	A	C6-N6	16.86	1.47	1.33
26	BA	1156	A	C6-N6	16.86	1.47	1.33
26	BA	1287	A	C6-N6	16.86	1.47	1.33
26	BA	1802	A	C6-N6	16.86	1.47	1.33
26	BA	1978	A	C6-N6	16.86	1.47	1.33
26	BA	2060	A	C6-N6	16.86	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2173	A	C6-N6	16.86	1.47	1.33
26	BA	2336	A	C6-N6	16.86	1.47	1.33
26	BA	2534	A	C6-N6	16.86	1.47	1.33
1	AA	143	A	C6-N6	16.86	1.47	1.33
1	AA	533	A	C6-N6	16.86	1.47	1.33
1	AA	729	A	C6-N6	16.86	1.47	1.33
1	AA	807	A	C6-N6	16.86	1.47	1.33
1	AA	974	A	C6-N6	16.86	1.47	1.33
24	AX	9	A	C6-N6	16.86	1.47	1.33
26	BA	161	A	C6-N6	16.86	1.47	1.33
26	BA	223	A	C6-N6	16.86	1.47	1.33
26	BA	256	A	C6-N6	16.86	1.47	1.33
26	BA	348	A	C6-N6	16.86	1.47	1.33
26	BA	466	A	C6-N6	16.86	1.47	1.33
26	BA	592	A	C6-N6	16.86	1.47	1.33
26	BA	825	A	C6-N6	16.86	1.47	1.33
26	BA	925	A	C6-N6	16.86	1.47	1.33
26	BA	1669	A	C6-N6	16.86	1.47	1.33
26	BA	1900	A	C6-N6	16.86	1.47	1.33
26	BA	2433	A	C6-N6	16.86	1.47	1.33
1	AA	3	A	C6-N6	16.86	1.47	1.33
26	BA	443	A	C6-N6	16.86	1.47	1.33
26	BA	878	A	C6-N6	16.86	1.47	1.33
26	BA	1885	A	C6-N6	16.86	1.47	1.33
26	BA	2376	A	C6-N6	16.86	1.47	1.33
1	AA	32	A	C6-N6	16.86	1.47	1.33
1	AA	149	A	C6-N6	16.86	1.47	1.33
1	AA	236	A	C6-N6	16.86	1.47	1.33
1	AA	336	A	C6-N6	16.86	1.47	1.33
1	AA	579	A	C6-N6	16.86	1.47	1.33
1	AA	914	A	C6-N6	16.86	1.47	1.33
1	AA	1362	A	C6-N6	16.86	1.47	1.33
26	BA	94	A	C6-N6	16.86	1.47	1.33
26	BA	300	A	C6-N6	16.86	1.47	1.33
26	BA	404	A	C6-N6	16.86	1.47	1.33
26	BA	716	A	C6-N6	16.86	1.47	1.33
26	BA	1383	A	C6-N6	16.86	1.47	1.33
26	BA	1549	A	C6-N6	16.86	1.47	1.33
26	BA	1610	A	C6-N6	16.86	1.47	1.33
26	BA	1676	A	C6-N6	16.86	1.47	1.33
26	BA	2600	A	C6-N6	16.86	1.47	1.33
26	BA	2660	A	C6-N6	16.86	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2749	A	C6-N6	16.86	1.47	1.33
1	AA	878	A	C6-N6	16.86	1.47	1.33
24	AX	41	A	C6-N6	16.86	1.47	1.33
26	BA	391	A	C6-N6	16.86	1.47	1.33
26	BA	793	A	C6-N6	16.86	1.47	1.33
26	BA	802	A	C6-N6	16.86	1.47	1.33
26	BA	1632	A	C6-N6	16.86	1.47	1.33
26	BA	1745	A	C6-N6	16.86	1.47	1.33
26	BA	1786	A	C6-N6	16.86	1.47	1.33
26	BA	2448	A	C6-N6	16.86	1.47	1.33
1	AA	161	A	C6-N6	16.85	1.47	1.33
1	AA	968	A	C6-N6	16.85	1.47	1.33
1	AA	1251	A	C6-N6	16.85	1.47	1.33
1	AA	1340	A	C6-N6	16.85	1.47	1.33
1	AA	1446	A	C6-N6	16.85	1.47	1.33
23	AW	31	A	C6-N6	16.85	1.47	1.33
26	BA	233	A	C6-N6	16.85	1.47	1.33
26	BA	788	A	C6-N6	16.85	1.47	1.33
26	BA	1347	A	C6-N6	16.85	1.47	1.33
26	BA	1698	A	C6-N6	16.85	1.47	1.33
26	BA	1791	A	C6-N6	16.85	1.47	1.33
1	AA	949	A	C6-N6	16.85	1.47	1.33
22	AV	21	A	C6-N6	16.85	1.47	1.33
26	BA	1439	A	C6-N6	16.85	1.47	1.33
26	BA	1525	A	C6-N6	16.85	1.47	1.33
26	BA	1616	A	C6-N6	16.85	1.47	1.33
26	BA	2119	A	C6-N6	16.85	1.47	1.33
26	BA	2531	A	C6-N6	16.85	1.47	1.33
26	BA	2598	A	C6-N6	16.85	1.47	1.33
1	AA	274	A	C6-N6	16.85	1.47	1.33
1	AA	288	A	C6-N6	16.85	1.47	1.33
1	AA	520	A	C6-N6	16.85	1.47	1.33
1	AA	635	A	C6-N6	16.85	1.47	1.33
1	AA	728	A	C6-N6	16.85	1.47	1.33
1	AA	1046	A	C6-N6	16.85	1.47	1.33
1	AA	1252	A	C6-N6	16.85	1.47	1.33
1	AA	1332	A	C6-N6	16.85	1.47	1.33
1	AA	1493	A	C6-N6	16.85	1.47	1.33
24	AX	3	A	C6-N6	16.85	1.47	1.33
25	AY	23	A	C6-N6	16.85	1.47	1.33
26	BA	244	A	C6-N6	16.85	1.47	1.33
26	BA	384	A	C6-N6	16.85	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	472	A	C6-N6	16.85	1.47	1.33
26	BA	501	A	C6-N6	16.85	1.47	1.33
26	BA	538	A	C6-N6	16.85	1.47	1.33
26	BA	789	A	C6-N6	16.85	1.47	1.33
26	BA	1020	A	C6-N6	16.85	1.47	1.33
26	BA	1067	A	C6-N6	16.85	1.47	1.33
26	BA	1260	A	C6-N6	16.85	1.47	1.33
26	BA	1477	A	C6-N6	16.85	1.47	1.33
26	BA	1677	A	C6-N6	16.85	1.47	1.33
26	BA	1690	A	C6-N6	16.85	1.47	1.33
26	BA	1717	A	C6-N6	16.85	1.47	1.33
1	AA	1503	A	C6-N6	16.85	1.47	1.33
26	BA	262	A	C6-N6	16.85	1.47	1.33
26	BA	927	A	C6-N6	16.85	1.47	1.33
26	BA	1050	A	C6-N6	16.85	1.47	1.33
26	BA	1634	A	C6-N6	16.85	1.47	1.33
26	BA	1815	A	C6-N6	16.85	1.47	1.33
26	BA	2738	A	C6-N6	16.85	1.47	1.33
1	AA	523	A	C6-N6	16.85	1.47	1.33
1	AA	918	A	C6-N6	16.85	1.47	1.33
1	AA	1236	A	C6-N6	16.85	1.47	1.33
23	AW	23	A	C6-N6	16.85	1.47	1.33
26	BA	428	A	C6-N6	16.85	1.47	1.33
26	BA	1254	A	C6-N6	16.85	1.47	1.33
26	BA	1572	A	C6-N6	16.85	1.47	1.33
26	BA	1598	A	C6-N6	16.85	1.47	1.33
26	BA	2126	A	C6-N6	16.85	1.47	1.33
26	BA	2147	A	C6-N6	16.85	1.47	1.33
26	BA	2377	A	C6-N6	16.85	1.47	1.33
26	BA	2868	A	C6-N6	16.85	1.47	1.33
26	BA	782	A	C6-N6	16.85	1.47	1.33
26	BA	1762	A	C6-N6	16.85	1.47	1.33
1	AA	279	A	C6-N6	16.84	1.47	1.33
1	AA	461	A	C6-N6	16.84	1.47	1.33
1	AA	1022	A	C6-N6	16.84	1.47	1.33
1	AA	1155	A	C6-N6	16.84	1.47	1.33
1	AA	1254	A	C6-N6	16.84	1.47	1.33
23	AW	14	A	C6-N6	16.84	1.47	1.33
26	BA	167	A	C6-N6	16.84	1.47	1.33
26	BA	1307	A	C6-N6	16.84	1.47	1.33
26	BA	1308	A	C6-N6	16.84	1.47	1.33
26	BA	1470	A	C6-N6	16.84	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1528	A	C6-N6	16.84	1.47	1.33
26	BA	1618	A	C6-N6	16.84	1.47	1.33
26	BA	1794	A	C6-N6	16.84	1.47	1.33
26	BA	1819	A	C6-N6	16.84	1.47	1.33
26	BA	2288	A	C6-N6	16.84	1.47	1.33
26	BA	2614	A	C6-N6	16.84	1.47	1.33
27	BB	109	A	C6-N6	16.84	1.47	1.33
27	BB	119	A	C6-N6	16.84	1.47	1.33
1	AA	1229	A	C6-N6	16.84	1.47	1.33
26	BA	981	A	C6-N6	16.84	1.47	1.33
26	BA	1301	A	C6-N6	16.84	1.47	1.33
26	BA	1502	A	C6-N6	16.84	1.47	1.33
26	BA	2412	A	C6-N6	16.84	1.47	1.33
26	BA	2566	A	C6-N6	16.84	1.47	1.33
1	AA	1055	A	C6-N6	16.84	1.47	1.33
1	AA	1447	A	C6-N6	16.84	1.47	1.33
23	AW	38	A	C6-N6	16.84	1.47	1.33
26	BA	492	A	C6-N6	16.84	1.47	1.33
26	BA	547	A	C6-N6	16.84	1.47	1.33
26	BA	866	A	C6-N6	16.84	1.47	1.33
26	BA	1046	A	C6-N6	16.84	1.47	1.33
26	BA	1342	A	C6-N6	16.84	1.47	1.33
26	BA	1637	A	C6-N6	16.84	1.47	1.33
26	BA	1739	A	C6-N6	16.84	1.47	1.33
26	BA	2406	A	C6-N6	16.84	1.47	1.33
26	BA	2425	A	C6-N6	16.84	1.47	1.33
1	AA	10	A	C6-N6	16.84	1.47	1.33
1	AA	120	A	C6-N6	16.84	1.47	1.33
1	AA	655	A	C6-N6	16.84	1.47	1.33
1	AA	906	A	C6-N6	16.84	1.47	1.33
1	AA	1508	A	C6-N6	16.84	1.47	1.33
25	AY	6	A	C6-N6	16.84	1.47	1.33
26	BA	226	A	C6-N6	16.84	1.47	1.33
26	BA	1321	A	C6-N6	16.84	1.47	1.33
26	BA	1803	A	C6-N6	16.84	1.47	1.33
26	BA	2886	A	C6-N6	16.84	1.47	1.33
1	AA	139	A	C6-N6	16.84	1.47	1.33
1	AA	1492	A	C6-N6	16.84	1.47	1.33
23	AW	21	A	C6-N6	16.84	1.47	1.33
26	BA	131	A	C6-N6	16.84	1.47	1.33
26	BA	412	A	C6-N6	16.84	1.47	1.33
26	BA	896	A	C6-N6	16.84	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2170	A	C6-N6	16.84	1.47	1.33
1	AA	712	A	C6-N6	16.84	1.47	1.33
1	AA	792	A	C6-N6	16.84	1.47	1.33
26	BA	1789	A	C6-N6	16.84	1.47	1.33
1	AA	174	A	C6-N6	16.84	1.47	1.33
1	AA	189	A	C6-N6	16.84	1.47	1.33
1	AA	509	A	C6-N6	16.84	1.47	1.33
1	AA	673	A	C6-N6	16.84	1.47	1.33
1	AA	1465	A	C6-N6	16.84	1.47	1.33
25	AY	14	A	C6-N6	16.84	1.47	1.33
26	BA	5	A	C6-N6	16.84	1.47	1.33
26	BA	21	A	C6-N6	16.84	1.47	1.33
26	BA	918	A	C6-N6	16.84	1.47	1.33
26	BA	2020	A	C6-N6	16.84	1.47	1.33
27	BB	58	A	C6-N6	16.84	1.47	1.33
1	AA	1288	A	C6-N6	16.83	1.47	1.33
26	BA	996	A	C6-N6	16.83	1.47	1.33
26	BA	1057	A	C6-N6	16.83	1.47	1.33
26	BA	1354	A	C6-N6	16.83	1.47	1.33
26	BA	1420	A	C6-N6	16.83	1.47	1.33
26	BA	1722	A	C6-N6	16.83	1.47	1.33
26	BA	2163	A	C6-N6	16.83	1.47	1.33
27	BB	108	A	C6-N6	16.83	1.47	1.33
1	AA	55	A	C6-N6	16.83	1.47	1.33
1	AA	1035	A	C6-N6	16.83	1.47	1.33
26	BA	152	A	C6-N6	16.83	1.47	1.33
26	BA	221	A	C6-N6	16.83	1.47	1.33
26	BA	371	A	C6-N6	16.83	1.47	1.33
26	BA	382	A	C6-N6	16.83	1.47	1.33
26	BA	616	A	C6-N6	16.83	1.47	1.33
26	BA	670	A	C6-N6	16.83	1.47	1.33
26	BA	743	A	C6-N6	16.83	1.47	1.33
26	BA	820	A	C6-N6	16.83	1.47	1.33
26	BA	1089	A	C6-N6	16.83	1.47	1.33
26	BA	2211	A	C6-N6	16.83	1.47	1.33
26	BA	2411	A	C6-N6	16.83	1.47	1.33
26	BA	2711	A	C6-N6	16.83	1.47	1.33
26	BA	2734	A	C6-N6	16.83	1.47	1.33
26	BA	2882	A	C6-N6	16.83	1.47	1.33
1	AA	262	A	C6-N6	16.83	1.47	1.33
1	AA	303	A	C6-N6	16.83	1.47	1.33
1	AA	465	A	C6-N6	16.83	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	768	A	C6-N6	16.83	1.47	1.33
1	AA	1363	A	C6-N6	16.83	1.47	1.33
26	BA	2059	A	C6-N6	16.83	1.47	1.33
26	BA	2706	A	C6-N6	16.83	1.47	1.33
1	AA	172	A	C6-N6	16.83	1.47	1.33
1	AA	195	A	C6-N6	16.83	1.47	1.33
1	AA	321	A	C6-N6	16.83	1.47	1.33
1	AA	371	A	C6-N6	16.83	1.47	1.33
1	AA	435	A	C6-N6	16.83	1.47	1.33
1	AA	535	A	C6-N6	16.83	1.47	1.33
26	BA	216	A	C6-N6	16.83	1.47	1.33
26	BA	941	A	C6-N6	16.83	1.47	1.33
26	BA	988	A	C6-N6	16.83	1.47	1.33
26	BA	1504	A	C6-N6	16.83	1.47	1.33
26	BA	1635	A	C6-N6	16.83	1.47	1.33
26	BA	1821	A	C6-N6	16.83	1.47	1.33
26	BA	1919	A	C6-N6	16.83	1.47	1.33
1	AA	182	A	C6-N6	16.83	1.47	1.33
1	AA	383	A	C6-N6	16.83	1.47	1.33
1	AA	964	A	C6-N6	16.83	1.47	1.33
1	AA	1180	A	C6-N6	16.83	1.47	1.33
26	BA	146	A	C6-N6	16.83	1.47	1.33
26	BA	362	A	C6-N6	16.83	1.47	1.33
26	BA	541	A	C6-N6	16.83	1.47	1.33
26	BA	626	A	C6-N6	16.83	1.47	1.33
26	BA	973	A	C6-N6	16.83	1.47	1.33
26	BA	1096	A	C6-N6	16.83	1.47	1.33
26	BA	1640	A	C6-N6	16.83	1.47	1.33
26	BA	1853	A	C6-N6	16.83	1.47	1.33
26	BA	2883	A	C6-N6	16.83	1.47	1.33
26	BA	2900	A	C6-N6	16.83	1.47	1.33
1	AA	539	A	C6-N6	16.83	1.47	1.33
26	BA	508	A	C6-N6	16.83	1.47	1.33
26	BA	689	A	C6-N6	16.83	1.47	1.33
26	BA	1264	A	C6-N6	16.83	1.47	1.33
26	BA	2369	A	C6-N6	16.83	1.47	1.33
26	BA	2733	A	C6-N6	16.83	1.47	1.33
26	BA	2826	A	C6-N6	16.83	1.47	1.33
1	AA	53	A	C6-N6	16.82	1.47	1.33
1	AA	327	A	C6-N6	16.82	1.47	1.33
1	AA	344	A	C6-N6	16.82	1.47	1.33
1	AA	364	A	C6-N6	16.82	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	19	A	C6-N6	16.82	1.47	1.33
26	BA	374	A	C6-N6	16.82	1.47	1.33
26	BA	502	A	C6-N6	16.82	1.47	1.33
26	BA	705	A	C6-N6	16.82	1.47	1.33
26	BA	706	A	C6-N6	16.82	1.47	1.33
26	BA	1048	A	C6-N6	16.82	1.47	1.33
26	BA	1678	A	C6-N6	16.82	1.47	1.33
26	BA	2070	A	C6-N6	16.82	1.47	1.33
26	BA	2451	A	C6-N6	16.82	1.47	1.33
26	BA	2503	A	C6-N6	16.82	1.47	1.33
1	AA	996	A	C6-N6	16.82	1.47	1.33
1	AA	1012	A	C6-N6	16.82	1.47	1.33
26	BA	574	A	C6-N6	16.82	1.47	1.33
26	BA	1509	A	C6-N6	16.82	1.47	1.33
26	BA	1665	A	C6-N6	16.82	1.47	1.33
26	BA	1916	A	C6-N6	16.82	1.47	1.33
26	BA	2095	A	C6-N6	16.82	1.47	1.33
1	AA	26	A	C6-N6	16.82	1.47	1.33
1	AA	28	A	C6-N6	16.82	1.47	1.33
1	AA	482	A	C6-N6	16.82	1.47	1.33
1	AA	595	A	C6-N6	16.82	1.47	1.33
26	BA	6	A	C6-N6	16.82	1.47	1.33
26	BA	149	A	C6-N6	16.82	1.47	1.33
26	BA	197	A	C6-N6	16.82	1.47	1.33
26	BA	251	A	C6-N6	16.82	1.47	1.33
26	BA	483	A	C6-N6	16.82	1.47	1.33
26	BA	515	A	C6-N6	16.82	1.47	1.33
26	BA	1085	A	C6-N6	16.82	1.47	1.33
26	BA	1854	A	C6-N6	16.82	1.47	1.33
26	BA	2134	A	C6-N6	16.82	1.47	1.33
27	BB	39	A	C6-N6	16.82	1.47	1.33
1	AA	459	A	C6-N6	16.82	1.47	1.33
1	AA	1250	A	C6-N6	16.82	1.47	1.33
26	BA	294	A	C6-N6	16.82	1.47	1.33
26	BA	2241	A	C6-N6	16.82	1.47	1.33
1	AA	160	A	C6-N6	16.82	1.47	1.33
1	AA	621	A	C6-N6	16.82	1.47	1.33
1	AA	718	A	C6-N6	16.82	1.47	1.33
1	AA	777	A	C6-N6	16.82	1.47	1.33
1	AA	919	A	C6-N6	16.82	1.47	1.33
1	AA	1216	A	C6-N6	16.82	1.47	1.33
22	AV	15	A	C6-N6	16.82	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	599	A	C6-N6	16.82	1.47	1.33
26	BA	1253	A	C6-N6	16.82	1.47	1.33
26	BA	1544	A	C6-N6	16.82	1.47	1.33
26	BA	1586	A	C6-N6	16.82	1.47	1.33
26	BA	1829	A	C6-N6	16.82	1.47	1.33
26	BA	1876	A	C6-N6	16.82	1.47	1.33
26	BA	2247	A	C6-N6	16.82	1.47	1.33
26	BA	2727	A	C6-N6	16.82	1.47	1.33
26	BA	172	A	C6-N6	16.82	1.47	1.33
26	BA	761	A	C6-N6	16.82	1.47	1.33
26	BA	975	A	C6-N6	16.82	1.47	1.33
26	BA	1084	A	C6-N6	16.82	1.47	1.33
26	BA	1548	A	C6-N6	16.82	1.47	1.33
26	BA	1569	A	C6-N6	16.82	1.47	1.33
26	BA	2278	A	C6-N6	16.82	1.47	1.33
1	AA	583	A	C6-N6	16.82	1.47	1.33
1	AA	938	A	C6-N6	16.82	1.47	1.33
1	AA	1105	A	C6-N6	16.82	1.47	1.33
26	BA	311	A	C6-N6	16.82	1.47	1.33
26	BA	332	A	C6-N6	16.82	1.47	1.33
26	BA	677	A	C6-N6	16.81	1.47	1.33
26	BA	2799	A	C6-N6	16.81	1.47	1.33
1	AA	109	A	C6-N6	16.81	1.47	1.33
1	AA	151	A	C6-N6	16.81	1.47	1.33
1	AA	642	A	C6-N6	16.81	1.47	1.33
1	AA	794	A	C6-N6	16.81	1.47	1.33
26	BA	621	A	C6-N6	16.81	1.47	1.33
26	BA	1088	A	C6-N6	16.81	1.47	1.33
26	BA	1614	A	C6-N6	16.81	1.47	1.33
26	BA	2077	A	C6-N6	16.81	1.47	1.33
26	BA	2212	A	C6-N6	16.81	1.47	1.33
26	BA	2682	A	C6-N6	16.81	1.47	1.33
1	AA	716	A	C6-N6	16.81	1.47	1.33
26	BA	1787	A	C6-N6	16.81	1.47	1.33
1	AA	975	A	C6-N6	16.81	1.47	1.33
1	AA	1044	A	C6-N6	16.81	1.47	1.33
26	BA	756	A	C6-N6	16.81	1.47	1.33
26	BA	1143	A	C6-N6	16.81	1.47	1.33
26	BA	1977	A	C6-N6	16.81	1.47	1.33
26	BA	2037	A	C6-N6	16.81	1.47	1.33
26	BA	2199	A	C6-N6	16.81	1.47	1.33
1	AA	33	A	C6-N6	16.81	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	238	A	C6-N6	16.81	1.47	1.33
1	AA	706	A	C6-N6	16.81	1.47	1.33
26	BA	735	A	C6-N6	16.81	1.47	1.33
26	BA	936	A	C6-N6	16.81	1.47	1.33
26	BA	1230	A	C6-N6	16.81	1.47	1.33
26	BA	2497	A	C6-N6	16.81	1.47	1.33
1	AA	306	A	C6-N6	16.81	1.47	1.33
1	AA	1377	A	C6-N6	16.81	1.47	1.33
24	AX	58	A	C6-N6	16.81	1.47	1.33
25	AY	21	A	C6-N6	16.81	1.47	1.33
26	BA	928	A	C6-N6	16.81	1.47	1.33
26	BA	1009	A	C6-N6	16.81	1.47	1.33
26	BA	1265	A	C6-N6	16.81	1.47	1.33
26	BA	1608	A	C6-N6	16.81	1.47	1.33
26	BA	2328	A	C6-N6	16.81	1.47	1.33
26	BA	2757	A	C6-N6	16.81	1.47	1.33
26	BA	2879	A	C6-N6	16.81	1.47	1.33
27	BB	94	A	C6-N6	16.81	1.47	1.33
1	AA	8	A	C6-N6	16.80	1.47	1.33
1	AA	356	A	C6-N6	16.80	1.47	1.33
1	AA	1171	A	C6-N6	16.80	1.47	1.33
1	AA	1269	A	C6-N6	16.80	1.47	1.33
26	BA	13	A	C6-N6	16.80	1.47	1.33
26	BA	84	A	C6-N6	16.80	1.47	1.33
26	BA	637	A	C6-N6	16.80	1.47	1.33
26	BA	722	A	C6-N6	16.80	1.47	1.33
26	BA	1032	A	C6-N6	16.80	1.47	1.33
26	BA	1111	A	C6-N6	16.80	1.47	1.33
26	BA	1387	A	C6-N6	16.80	1.47	1.33
1	AA	600	A	C6-N6	16.80	1.47	1.33
1	AA	665	A	C6-N6	16.80	1.47	1.33
1	AA	753	A	C6-N6	16.80	1.47	1.33
26	BA	71	A	C6-N6	16.80	1.47	1.33
26	BA	255	A	C6-N6	16.80	1.47	1.33
26	BA	602	A	C6-N6	16.80	1.47	1.33
26	BA	721	A	C6-N6	16.80	1.47	1.33
26	BA	730	A	C6-N6	16.80	1.47	1.33
26	BA	911	A	C6-N6	16.80	1.47	1.33
26	BA	1705	A	C6-N6	16.80	1.47	1.33
26	BA	1889	A	C6-N6	16.80	1.47	1.33
26	BA	1936	A	C6-N6	16.80	1.47	1.33
26	BA	2541	A	C6-N6	16.80	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BB	99	A	C6-N6	16.80	1.47	1.33
27	BB	115	A	C6-N6	16.80	1.47	1.33
1	AA	546	A	C6-N6	16.80	1.47	1.33
1	AA	602	A	C6-N6	16.80	1.47	1.33
1	AA	629	A	C6-N6	16.80	1.47	1.33
1	AA	1394	A	C6-N6	16.80	1.47	1.33
1	AA	630	A	C6-N6	16.80	1.47	1.33
1	AA	663	A	C6-N6	16.80	1.47	1.33
1	AA	1238	A	C6-N6	16.80	1.47	1.33
1	AA	1456	A	C6-N6	16.80	1.47	1.33
26	BA	218	A	C6-N6	16.80	1.47	1.33
26	BA	1713	A	C6-N6	16.80	1.47	1.33
1	AA	1299	A	C6-N6	16.80	1.47	1.33
26	BA	73	A	C6-N6	16.80	1.47	1.33
26	BA	270	A	C6-N6	16.80	1.47	1.33
26	BA	2657	A	C6-N6	16.80	1.47	1.33
26	BA	2765	A	C6-N6	16.80	1.47	1.33
26	BA	2873	A	C6-N6	16.80	1.47	1.33
1	AA	937	A	C6-N6	16.80	1.47	1.33
26	BA	613	A	C6-N6	16.80	1.47	1.33
26	BA	715	A	C6-N6	16.80	1.47	1.33
26	BA	752	A	C6-N6	16.80	1.47	1.33
26	BA	877	A	C6-N6	16.80	1.47	1.33
26	BA	1532	A	C6-N6	16.80	1.47	1.33
26	BA	1609	A	C6-N6	16.80	1.47	1.33
26	BA	2432	A	C6-N6	16.80	1.47	1.33
26	BA	2461	A	C6-N6	16.80	1.47	1.33
26	BA	2516	A	C6-N6	16.80	1.47	1.33
1	AA	1081	A	C6-N6	16.80	1.47	1.33
1	AA	1082	A	C6-N6	16.80	1.47	1.33
1	AA	1163	A	C6-N6	16.80	1.47	1.33
26	BA	1579	A	C6-N6	16.80	1.47	1.33
26	BA	1809	A	C6-N6	16.80	1.47	1.33
26	BA	2471	A	C6-N6	16.80	1.47	1.33
27	BB	45	A	C6-N6	16.80	1.47	1.33
26	BA	1275	A	C6-N6	16.79	1.47	1.33
26	BA	1650	A	C6-N6	16.79	1.47	1.33
1	AA	573	A	C6-N6	16.79	1.47	1.33
1	AA	969	A	C6-N6	16.79	1.47	1.33
1	AA	1067	A	C6-N6	16.79	1.47	1.33
1	AA	1191	A	C6-N6	16.79	1.47	1.33
1	AA	1196	A	C6-N6	16.79	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1127	A	C6-N6	16.79	1.47	1.33
26	BA	1247	A	C6-N6	16.79	1.47	1.33
26	BA	2184	A	C6-N6	16.79	1.47	1.33
26	BA	2268	A	C6-N6	16.79	1.47	1.33
26	BA	2327	A	C6-N6	16.79	1.47	1.33
1	AA	696	A	C6-N6	16.79	1.47	1.33
26	BA	144	A	C6-N6	16.79	1.47	1.33
26	BA	423	A	C6-N6	16.79	1.47	1.33
26	BA	1000	A	C6-N6	16.79	1.47	1.33
26	BA	1142	A	C6-N6	16.79	1.47	1.33
1	AA	909	A	C6-N6	16.79	1.47	1.33
1	AA	1434	A	C6-N6	16.79	1.47	1.33
26	BA	532	A	C6-N6	16.79	1.47	1.33
26	BA	1654	A	C6-N6	16.79	1.47	1.33
26	BA	2015	A	C6-N6	16.79	1.47	1.33
1	AA	1201	A	C6-N6	16.79	1.47	1.33
26	BA	265	A	C6-N6	16.79	1.47	1.33
26	BA	1098	A	C6-N6	16.79	1.47	1.33
26	BA	1272	A	C6-N6	16.79	1.47	1.33
26	BA	1327	A	C6-N6	16.79	1.47	1.33
26	BA	2298	A	C6-N6	16.79	1.47	1.33
26	BA	2572	A	C6-N6	16.79	1.47	1.33
1	AA	759	A	C6-N6	16.79	1.47	1.33
1	AA	802	A	C6-N6	16.79	1.47	1.33
1	AA	1213	A	C6-N6	16.79	1.47	1.33
1	AA	1431	A	C6-N6	16.79	1.47	1.33
26	BA	182	A	C6-N6	16.79	1.47	1.33
26	BA	241	A	C6-N6	16.79	1.47	1.33
26	BA	278	A	C6-N6	16.79	1.47	1.33
26	BA	608	A	C6-N6	16.79	1.47	1.33
26	BA	1427	A	C6-N6	16.79	1.47	1.33
26	BA	2726	A	C6-N6	16.79	1.47	1.33
27	BB	66	A	C6-N6	16.79	1.47	1.33
24	AX	23	A	C6-N6	16.79	1.47	1.33
26	BA	675	A	C6-N6	16.79	1.47	1.33
26	BA	1434	A	C6-N6	16.79	1.47	1.33
26	BA	1689	A	C6-N6	16.79	1.47	1.33
26	BA	2386	A	C6-N6	16.79	1.47	1.33
1	AA	782	A	C6-N6	16.78	1.47	1.33
1	AA	1117	A	C6-N6	16.78	1.47	1.33
26	BA	1378	A	C6-N6	16.78	1.47	1.33
26	BA	1603	A	C6-N6	16.78	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	408	A	C6-N6	16.78	1.47	1.33
1	AA	946	A	C6-N6	16.78	1.47	1.33
26	BA	2542	A	C6-N6	16.78	1.47	1.33
27	BB	52	A	C6-N6	16.78	1.47	1.33
1	AA	298	A	C6-N6	16.78	1.47	1.33
1	AA	325	A	C6-N6	16.78	1.47	1.33
26	BA	739	A	C6-N6	16.78	1.47	1.33
26	BA	990	A	C6-N6	16.78	1.47	1.33
26	BA	2158	A	C6-N6	16.78	1.47	1.33
1	AA	889	A	C6-N6	16.78	1.47	1.33
1	AA	1219	A	C6-N6	16.78	1.47	1.33
26	BA	800	A	C6-N6	16.78	1.47	1.33
26	BA	1392	A	C6-N6	16.78	1.47	1.33
1	AA	65	A	C6-N6	16.78	1.47	1.33
1	AA	130	A	C6-N6	16.78	1.47	1.33
26	BA	861	A	C6-N6	16.78	1.47	1.33
26	BA	1155	A	C6-N6	16.78	1.47	1.33
26	BA	1359	A	C6-N6	16.78	1.47	1.33
26	BA	1626	A	C6-N6	16.78	1.47	1.33
26	BA	1759	A	C6-N6	16.78	1.47	1.33
26	BA	1735	A	C6-N6	16.78	1.47	1.33
26	BA	1805	A	C6-N6	16.78	1.47	1.33
1	AA	452	A	C6-N6	16.77	1.47	1.33
1	AA	915	A	C6-N6	16.77	1.47	1.33
1	AA	1289	A	C6-N6	16.77	1.47	1.33
26	BA	95	A	C6-N6	16.77	1.47	1.33
26	BA	222	A	C6-N6	16.77	1.47	1.33
26	BA	346	A	C6-N6	16.77	1.47	1.33
26	BA	460	A	C6-N6	16.77	1.47	1.33
1	AA	205	A	C6-N6	16.77	1.47	1.33
1	AA	1333	A	C6-N6	16.77	1.47	1.33
26	BA	1591	A	C6-N6	16.77	1.47	1.33
1	AA	374	A	C6-N6	16.77	1.47	1.33
1	AA	784	A	C6-N6	16.77	1.47	1.33
1	AA	1476	A	C6-N6	16.77	1.47	1.33
25	AY	38	A	C6-N6	16.77	1.47	1.33
26	BA	676	A	C6-N6	16.77	1.47	1.33
26	BA	1494	A	C6-N6	16.77	1.47	1.33
26	BA	2088	A	C6-N6	16.77	1.47	1.33
26	BA	2810	A	C6-N6	16.77	1.47	1.33
26	BA	563	A	C6-N6	16.77	1.47	1.33
26	BA	1877	A	C6-N6	16.77	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	199	A	C6-N6	16.77	1.47	1.33
1	AA	1170	A	C6-N6	16.77	1.47	1.33
1	AA	1324	A	C6-N6	16.77	1.47	1.33
1	AA	1430	A	C6-N6	16.77	1.47	1.33
26	BA	526	A	C6-N6	16.77	1.47	1.33
26	BA	2565	A	C6-N6	16.77	1.47	1.33
1	AA	1021	A	C6-N6	16.77	1.47	1.33
1	AA	1357	A	C6-N6	16.77	1.47	1.33
26	BA	2560	A	C6-N6	16.77	1.47	1.33
26	BA	2835	A	C6-N6	16.77	1.47	1.33
27	BB	53	A	C6-N6	16.77	1.47	1.33
1	AA	766	A	C6-N6	16.77	1.47	1.33
26	BA	324	A	C6-N6	16.77	1.47	1.33
26	BA	783	A	C6-N6	16.77	1.47	1.33
26	BA	1269	A	C6-N6	16.77	1.47	1.33
26	BA	2478	A	C6-N6	16.77	1.47	1.33
26	BA	207	A	C6-N6	16.76	1.47	1.33
26	BA	522	A	C6-N6	16.76	1.47	1.33
1	AA	382	A	C6-N6	16.76	1.47	1.33
1	AA	460	A	C6-N6	16.76	1.47	1.33
1	AA	1285	A	C6-N6	16.76	1.47	1.33
1	AA	1518	A	C6-N6	16.76	1.47	1.33
26	BA	586	A	C6-N6	16.76	1.47	1.33
26	BA	920	A	C6-N6	16.76	1.47	1.33
26	BA	1328	A	C6-N6	16.76	1.47	1.33
26	BA	1783	A	C6-N6	16.76	1.47	1.33
26	BA	1901	A	C6-N6	16.76	1.47	1.33
26	BA	2820	A	C6-N6	16.76	1.47	1.33
26	BA	863	A	C6-N6	16.76	1.47	1.33
26	BA	1552	A	C6-N6	16.76	1.47	1.33
26	BA	2287	A	C6-N6	16.76	1.47	1.33
1	AA	814	A	C6-N6	16.76	1.47	1.33
26	BA	10	A	C6-N6	16.76	1.47	1.33
26	BA	449	A	C6-N6	16.76	1.47	1.33
26	BA	655	A	C6-N6	16.76	1.47	1.33
26	BA	1268	A	C6-N6	16.76	1.47	1.33
26	BA	1522	A	C6-N6	16.76	1.47	1.33
26	BA	1808	A	C6-N6	16.76	1.47	1.33
26	BA	1848	A	C6-N6	16.76	1.47	1.33
1	AA	1157	A	C6-N6	16.76	1.47	1.33
26	BA	804	A	C6-N6	16.76	1.47	1.33
26	BA	909	A	C6-N6	16.76	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	983	A	C6-N6	16.76	1.47	1.33
26	BA	2358	A	C6-N6	16.76	1.47	1.33
1	AA	451	A	C6-N6	16.75	1.47	1.33
1	AA	1429	A	C6-N6	16.75	1.47	1.33
26	BA	821	A	C6-N6	16.75	1.47	1.33
26	BA	2094	A	C6-N6	16.75	1.47	1.33
26	BA	2577	A	C6-N6	16.75	1.47	1.33
26	BA	2518	A	C6-N6	16.75	1.47	1.33
1	AA	119	A	C6-N6	16.75	1.47	1.33
1	AA	1349	A	C6-N6	16.75	1.47	1.33
26	BA	2764	A	C6-N6	16.75	1.47	1.33
1	AA	493	A	C6-N6	16.75	1.47	1.33
1	AA	872	A	C6-N6	16.75	1.47	1.33
26	BA	2169	A	C6-N6	16.75	1.47	1.33
1	AA	1350	A	C6-N6	16.75	1.47	1.33
26	BA	204	A	C6-N6	16.75	1.47	1.33
26	BA	643	A	C6-N6	16.75	1.47	1.33
1	AA	746	A	C6-N6	16.75	1.47	1.33
1	AA	923	A	C6-N6	16.75	1.47	1.33
26	BA	1028	A	C6-N6	16.75	1.47	1.33
1	AA	499	A	C6-N6	16.74	1.47	1.33
1	AA	695	A	C6-N6	16.74	1.47	1.33
26	BA	1664	A	C6-N6	16.74	1.47	1.33
25	AY	9	A	C6-N6	16.74	1.47	1.33
26	BA	1419	A	C6-N6	16.74	1.47	1.33
26	BA	2005	A	C6-N6	16.74	1.47	1.33
26	BA	2333	A	C6-N6	16.74	1.47	1.33
26	BA	2725	A	C6-N6	16.74	1.47	1.33
26	BA	1801	A	C6-N6	16.74	1.47	1.33
26	BA	415	A	C6-N6	16.74	1.47	1.33
26	BA	1773	A	C6-N6	16.74	1.47	1.33
26	BA	529	A	C6-N6	16.74	1.47	1.33
1	AA	81	A	C6-N6	16.74	1.47	1.33
1	AA	353	A	C6-N6	16.74	1.47	1.33
1	AA	1275	A	C6-N6	16.74	1.47	1.33
26	BA	1353	A	C6-N6	16.73	1.47	1.33
26	BA	320	A	C6-N6	16.73	1.47	1.33
26	BA	1566	A	C6-N6	16.73	1.47	1.33
26	BA	1668	A	C6-N6	16.73	1.47	1.33
26	BA	2700	A	C6-N6	16.73	1.47	1.33
26	BA	2740	A	C6-N6	16.73	1.47	1.33
26	BA	661	A	C6-N6	16.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	910	A	C6-N6	16.73	1.47	1.33
26	BA	750	A	C6-N6	16.73	1.47	1.33
26	BA	1431	A	C6-N6	16.73	1.47	1.33
26	BA	2547	A	C6-N6	16.73	1.47	1.33
26	BA	2225	A	C6-N6	16.73	1.47	1.33
1	AA	389	A	C6-N6	16.72	1.47	1.33
26	BA	794	A	C6-N6	16.72	1.47	1.33
26	BA	900	A	C6-N6	16.72	1.47	1.33
1	AA	98	A	C6-N6	16.72	1.47	1.33
1	AA	1167	A	C6-N6	16.72	1.47	1.33
26	BA	1244	A	C6-N6	16.72	1.47	1.33
26	BA	2346	A	C6-N6	16.72	1.47	1.33
1	AA	865	A	C6-N6	16.72	1.47	1.33
1	AA	1239	A	C6-N6	16.72	1.47	1.33
24	AX	76	A	C6-N6	16.72	1.47	1.33
26	BA	2267	A	C6-N6	16.72	1.47	1.33
26	BA	2450	A	C6-N6	16.72	1.47	1.33
26	BA	2459	A	C6-N6	16.72	1.47	1.33
26	BA	2766	A	C6-N6	16.72	1.47	1.33
26	BA	2335	A	C6-N6	16.71	1.47	1.33
26	BA	1226	A	C6-N6	16.71	1.47	1.33
24	AX	24	A	C6-N6	16.71	1.47	1.33
1	AA	622	A	C6-N6	16.71	1.47	1.33
1	AA	1145	A	C6-N6	16.71	1.47	1.33
1	AA	1152	A	C6-N6	16.71	1.47	1.33
26	BA	2080	A	C6-N6	16.71	1.47	1.33
27	BB	50	A	C6-N6	16.71	1.47	1.33
27	BB	78	A	C6-N6	16.71	1.47	1.33
26	BA	44	A	C6-N6	16.71	1.47	1.33
26	BA	503	A	C6-N6	16.71	1.47	1.33
26	BA	1655	A	C6-N6	16.71	1.47	1.33
26	BA	2741	A	C6-N6	16.71	1.47	1.33
26	BA	119	A	C6-N6	16.70	1.47	1.33
26	BA	330	A	C6-N6	16.70	1.47	1.33
27	BB	59	A	C6-N6	16.70	1.47	1.33
1	AA	553	A	C6-N6	16.70	1.47	1.33
26	BA	2675	A	C6-N6	16.70	1.47	1.33
26	BA	1001	A	C6-N6	16.70	1.47	1.33
26	BA	2052	A	C6-N6	16.70	1.47	1.33
26	BA	279	A	C6-N6	16.70	1.47	1.33
1	AA	864	A	C6-N6	16.69	1.47	1.33
26	BA	575	A	C6-N6	16.69	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	845	A	C6-N6	16.69	1.47	1.33
23	AW	9	A	C6-N6	16.69	1.47	1.33
1	AA	171	A	C6-N6	16.69	1.47	1.33
26	BA	227	A	C6-N6	16.69	1.47	1.33
26	BA	1189	A	C6-N6	16.69	1.47	1.33
1	AA	270	A	C6-N6	16.69	1.47	1.33
1	AA	397	A	C6-N6	16.68	1.47	1.33
1	AA	430	A	C6-N6	16.68	1.47	1.33
1	AA	596	A	C6-N6	16.68	1.47	1.33
26	BA	933	A	C6-N6	16.68	1.47	1.33
1	AA	502	A	C6-N6	16.68	1.47	1.33
26	BA	1515	A	C6-N6	16.68	1.47	1.33
26	BA	2388	A	C6-N6	16.68	1.47	1.33
26	BA	2639	A	C6-N6	16.68	1.47	1.33
26	BA	582	A	C6-N6	16.68	1.47	1.33
26	BA	1214	A	C6-N6	16.68	1.47	1.33
26	BA	56	A	C6-N6	16.67	1.47	1.33
26	BA	1784	A	C6-N6	16.67	1.47	1.33
1	AA	412	A	C6-N6	16.67	1.47	1.33
26	BA	457	A	C6-N6	16.67	1.47	1.33
26	BA	685	A	C6-N6	16.66	1.47	1.33
26	BA	644	A	C6-N6	16.66	1.47	1.33
26	BA	1276	A	C6-N6	16.66	1.47	1.33
26	BA	2856	A	C6-N6	16.65	1.47	1.33
1	AA	1151	A	C6-N6	16.65	1.47	1.33
26	BA	2054	A	C6-N6	16.64	1.47	1.33
1	AA	432	A	C6-N6	16.64	1.47	1.33
1	AA	478	A	C6-N6	16.64	1.47	1.33
26	BA	1496	A	C6-N6	16.64	1.47	1.33
1	AA	608	A	C6-N6	16.63	1.47	1.33
26	BA	1899	A	C6-N6	16.63	1.47	1.33
26	BA	572	A	C6-N6	16.62	1.47	1.33
26	BA	1545	A	C6-N6	16.62	1.47	1.33
26	BA	142	A	C6-N6	16.61	1.47	1.33
26	BA	2800	A	C6-N6	16.60	1.47	1.33
1	AA	1102	A	C6-N6	16.56	1.47	1.33
26	BA	53	A	C6-N6	16.55	1.47	1.33
26	BA	2469	A	C6-N6	16.54	1.47	1.33
1	AA	495	A	C6-N6	16.45	1.47	1.33
26	BA	514	A	C6-N6	16.41	1.47	1.33
24	AX	1	G	OP3-P	-10.58	1.48	1.61
24	AX	16	U	N1-C6	10.19	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	20	U	N1-C6	10.15	1.47	1.38
24	AX	19	U	N1-C6	10.14	1.47	1.38
24	AX	20	U	N1-C6	10.11	1.47	1.38
24	AX	20	U	C4-C5	9.42	1.52	1.43
23	AW	20	U	C4-C5	9.35	1.51	1.43
24	AX	19	U	C4-C5	9.34	1.51	1.43
24	AX	16	U	C4-C5	9.24	1.51	1.43
26	BA	1378	A	C8-N7	8.17	1.37	1.31
26	BA	2451	A	C8-N7	8.13	1.37	1.31
23	AW	75	C	O3'-P	8.09	1.70	1.61
1	AA	452	A	C8-N7	8.01	1.37	1.31
1	AA	622	A	C8-N7	8.00	1.37	1.31
26	BA	119	A	C8-N7	7.95	1.37	1.31
1	AA	1329	A	C8-N7	7.93	1.37	1.31
26	BA	1785	A	C8-N7	7.93	1.37	1.31
1	AA	889	A	C8-N7	7.92	1.37	1.31
1	AA	431	A	C8-N7	7.92	1.37	1.31
27	BB	34	A	C8-N7	7.92	1.37	1.31
1	AA	171	A	C8-N7	7.88	1.37	1.31
1	AA	151	A	C8-N7	7.88	1.37	1.31
1	AA	665	A	C8-N7	7.87	1.37	1.31
26	BA	2764	A	C8-N7	7.87	1.37	1.31
26	BA	2469	A	C8-N7	7.85	1.37	1.31
26	BA	1652	A	C8-N7	7.85	1.37	1.31
1	AA	766	A	C8-N7	7.83	1.37	1.31
1	AA	182	A	C8-N7	7.83	1.37	1.31
26	BA	1419	A	C8-N7	7.82	1.37	1.31
1	AA	1248	A	C8-N7	7.82	1.37	1.31
26	BA	207	A	C8-N7	7.81	1.37	1.31
26	BA	2033	A	C8-N7	7.81	1.37	1.31
26	BA	1155	A	C8-N7	7.81	1.37	1.31
27	BB	78	A	C8-N7	7.81	1.37	1.31
26	BA	905	A	C8-N7	7.80	1.37	1.31
1	AA	1151	A	C8-N7	7.80	1.37	1.31
26	BA	529	A	C8-N7	7.79	1.37	1.31
26	BA	1427	A	C8-N7	7.79	1.37	1.31
26	BA	526	A	C8-N7	7.78	1.36	1.31
26	BA	1040	A	C8-N7	7.78	1.36	1.31
26	BA	1545	A	C8-N7	7.78	1.36	1.31
26	BA	457	A	C8-N7	7.78	1.36	1.31
1	AA	499	A	C8-N7	7.78	1.36	1.31
23	AW	42	A	C8-N7	7.77	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1876	A	C8-N7	7.77	1.36	1.31
1	AA	456	A	C8-N7	7.77	1.36	1.31
26	BA	371	A	C8-N7	7.77	1.36	1.31
26	BA	2418	A	C8-N7	7.77	1.36	1.31
26	BA	783	A	C8-N7	7.77	1.36	1.31
26	BA	1385	A	C8-N7	7.76	1.36	1.31
26	BA	1522	A	C8-N7	7.76	1.36	1.31
23	AW	51	A	C8-N7	7.76	1.36	1.31
26	BA	2478	A	C8-N7	7.76	1.36	1.31
26	BA	2530	A	C8-N7	7.76	1.36	1.31
26	BA	204	A	C8-N7	7.75	1.36	1.31
26	BA	574	A	C8-N7	7.75	1.36	1.31
26	BA	320	A	C8-N7	7.75	1.36	1.31
26	BA	1359	A	C8-N7	7.75	1.36	1.31
22	AV	22	A	C8-N7	7.74	1.36	1.31
26	BA	38	A	C8-N7	7.74	1.36	1.31
26	BA	2589	A	C8-N7	7.74	1.36	1.31
1	AA	195	A	C8-N7	7.74	1.36	1.31
1	AA	223	A	C8-N7	7.74	1.36	1.31
1	AA	1289	A	C8-N7	7.74	1.36	1.31
26	BA	2450	A	C8-N7	7.74	1.36	1.31
1	AA	1238	A	C8-N7	7.74	1.36	1.31
23	AW	9	A	C8-N7	7.74	1.36	1.31
26	BA	844	A	C8-N7	7.74	1.36	1.31
26	BA	2101	A	C8-N7	7.74	1.36	1.31
26	BA	89	A	C8-N7	7.74	1.36	1.31
26	BA	621	A	C8-N7	7.74	1.36	1.31
1	AA	1246	A	C8-N7	7.73	1.36	1.31
26	BA	2009	A	C8-N7	7.73	1.36	1.31
1	AA	825	A	C8-N7	7.73	1.36	1.31
1	AA	1410	A	C8-N7	7.73	1.36	1.31
1	AA	1428	A	C8-N7	7.73	1.36	1.31
26	BA	1794	A	C8-N7	7.73	1.36	1.31
26	BA	2388	A	C8-N7	7.73	1.36	1.31
26	BA	909	A	C8-N7	7.73	1.36	1.31
1	AA	72	A	C8-N7	7.73	1.36	1.31
26	BA	1286	A	C8-N7	7.73	1.36	1.31
26	BA	2322	A	C8-N7	7.72	1.36	1.31
1	AA	139	A	C8-N7	7.72	1.36	1.31
1	AA	913	A	C8-N7	7.72	1.36	1.31
1	AA	1170	A	C8-N7	7.72	1.36	1.31
26	BA	1147	A	C8-N7	7.72	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	155	A	C8-N7	7.72	1.36	1.31
26	BA	1413	A	C8-N7	7.72	1.36	1.31
26	BA	1515	A	C8-N7	7.71	1.36	1.31
26	BA	2031	A	C8-N7	7.71	1.36	1.31
1	AA	196	A	C8-N7	7.71	1.36	1.31
1	AA	533	A	C8-N7	7.71	1.36	1.31
1	AA	655	A	C8-N7	7.71	1.36	1.31
1	AA	78	A	C8-N7	7.71	1.36	1.31
1	AA	1155	A	C8-N7	7.71	1.36	1.31
26	BA	1590	A	C8-N7	7.71	1.36	1.31
1	AA	44	A	C8-N7	7.71	1.36	1.31
1	AA	160	A	C8-N7	7.71	1.36	1.31
1	AA	243	A	C8-N7	7.71	1.36	1.31
26	BA	2241	A	C8-N7	7.71	1.36	1.31
27	BB	46	A	C8-N7	7.71	1.36	1.31
26	BA	825	A	C8-N7	7.71	1.36	1.31
26	BA	1918	A	C8-N7	7.71	1.36	1.31
26	BA	167	A	C8-N7	7.70	1.36	1.31
26	BA	800	A	C8-N7	7.70	1.36	1.31
26	BA	983	A	C8-N7	7.70	1.36	1.31
26	BA	1194	A	C8-N7	7.70	1.36	1.31
26	BA	2288	A	C8-N7	7.70	1.36	1.31
26	BA	2070	A	C8-N7	7.70	1.36	1.31
1	AA	309	A	C8-N7	7.70	1.36	1.31
26	BA	1641	A	C8-N7	7.70	1.36	1.31
26	BA	2761	A	C8-N7	7.70	1.36	1.31
26	BA	497	A	C8-N7	7.70	1.36	1.31
26	BA	340	A	C8-N7	7.70	1.36	1.31
1	AA	246	A	C8-N7	7.70	1.36	1.31
1	AA	315	A	C8-N7	7.70	1.36	1.31
26	BA	590	A	C8-N7	7.70	1.36	1.31
26	BA	1566	A	C8-N7	7.70	1.36	1.31
26	BA	2868	A	C8-N7	7.70	1.36	1.31
1	AA	909	A	C8-N7	7.69	1.36	1.31
26	BA	472	A	C8-N7	7.69	1.36	1.31
26	BA	637	A	C8-N7	7.69	1.36	1.31
26	BA	2030	A	C8-N7	7.69	1.36	1.31
1	AA	26	A	C8-N7	7.69	1.36	1.31
1	AA	74	A	C8-N7	7.69	1.36	1.31
1	AA	946	A	C8-N7	7.69	1.36	1.31
26	BA	1937	A	C8-N7	7.69	1.36	1.31
26	BA	2135	A	C8-N7	7.69	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2753	A	C8-N7	7.69	1.36	1.31
1	AA	1117	A	C8-N7	7.69	1.36	1.31
26	BA	1755	A	C8-N7	7.69	1.36	1.31
1	AA	66	A	C8-N7	7.69	1.36	1.31
1	AA	282	A	C8-N7	7.69	1.36	1.31
1	AA	914	A	C8-N7	7.69	1.36	1.31
1	AA	1000	A	C8-N7	7.69	1.36	1.31
26	BA	1111	A	C8-N7	7.69	1.36	1.31
26	BA	1913	A	C8-N7	7.69	1.36	1.31
26	BA	2225	A	C8-N7	7.69	1.36	1.31
26	BA	2829	A	C8-N7	7.69	1.36	1.31
26	BA	1690	A	C8-N7	7.69	1.36	1.31
1	AA	1333	A	C8-N7	7.68	1.36	1.31
26	BA	226	A	C8-N7	7.68	1.36	1.31
26	BA	1701	A	C8-N7	7.68	1.36	1.31
26	BA	1853	A	C8-N7	7.68	1.36	1.31
26	BA	2108	A	C8-N7	7.68	1.36	1.31
26	BA	2835	A	C8-N7	7.68	1.36	1.31
1	AA	493	A	C8-N7	7.68	1.36	1.31
1	AA	1311	A	C8-N7	7.68	1.36	1.31
23	AW	73	A	C8-N7	7.68	1.36	1.31
25	AY	73	A	C8-N7	7.68	1.36	1.31
26	BA	1230	A	C8-N7	7.68	1.36	1.31
26	BA	1336	A	C8-N7	7.68	1.36	1.31
1	AA	915	A	C8-N7	7.68	1.36	1.31
1	AA	1275	A	C8-N7	7.68	1.36	1.31
26	BA	1477	A	C8-N7	7.68	1.36	1.31
26	BA	2134	A	C8-N7	7.68	1.36	1.31
26	BA	2381	A	C8-N7	7.68	1.36	1.31
26	BA	2741	A	C8-N7	7.68	1.36	1.31
26	BA	2173	A	C8-N7	7.68	1.36	1.31
26	BA	2738	A	C8-N7	7.68	1.36	1.31
1	AA	753	A	C8-N7	7.68	1.36	1.31
27	BB	104	A	C8-N7	7.68	1.36	1.31
23	AW	76	A	C8-N7	7.67	1.36	1.31
26	BA	1014	A	C8-N7	7.67	1.36	1.31
26	BA	592	A	C8-N7	7.67	1.36	1.31
26	BA	1960	A	C8-N7	7.67	1.36	1.31
1	AA	681	A	C8-N7	7.67	1.36	1.31
1	AA	978	A	C8-N7	7.67	1.36	1.31
26	BA	480	A	C8-N7	7.67	1.36	1.31
26	BA	2314	A	C8-N7	7.67	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	303	A	C8-N7	7.67	1.36	1.31
1	AA	366	A	C8-N7	7.67	1.36	1.31
1	AA	1368	A	C8-N7	7.67	1.36	1.31
1	AA	1493	A	C8-N7	7.67	1.36	1.31
26	BA	1901	A	C8-N7	7.67	1.36	1.31
1	AA	415	A	C8-N7	7.67	1.36	1.31
26	BA	1095	A	C8-N7	7.67	1.36	1.31
26	BA	2274	A	C8-N7	7.67	1.36	1.31
1	AA	320	A	C8-N7	7.67	1.36	1.31
1	AA	1188	A	C8-N7	7.67	1.36	1.31
26	BA	973	A	C8-N7	7.67	1.36	1.31
1	AA	129	A	C8-N7	7.67	1.36	1.31
26	BA	878	A	C8-N7	7.67	1.36	1.31
26	BA	1772	A	C8-N7	7.67	1.36	1.31
26	BA	2003	A	C8-N7	7.67	1.36	1.31
1	AA	749	A	C8-N7	7.66	1.36	1.31
1	AA	1019	A	C8-N7	7.66	1.36	1.31
26	BA	2090	A	C8-N7	7.66	1.36	1.31
26	BA	2600	A	C8-N7	7.66	1.36	1.31
26	BA	354	A	C8-N7	7.66	1.36	1.31
26	BA	655	A	C8-N7	7.66	1.36	1.31
26	BA	1001	A	C8-N7	7.66	1.36	1.31
26	BA	1254	A	C8-N7	7.66	1.36	1.31
1	AA	152	A	C8-N7	7.66	1.36	1.31
1	AA	313	A	C8-N7	7.66	1.36	1.31
26	BA	346	A	C8-N7	7.66	1.36	1.31
26	BA	911	A	C8-N7	7.66	1.36	1.31
26	BA	1308	A	C8-N7	7.66	1.36	1.31
26	BA	1757	A	C8-N7	7.66	1.36	1.31
1	AA	411	A	C8-N7	7.66	1.36	1.31
26	BA	1098	A	C8-N7	7.66	1.36	1.31
26	BA	342	A	C8-N7	7.66	1.36	1.31
26	BA	1302	A	C8-N7	7.66	1.36	1.31
1	AA	131	A	C8-N7	7.66	1.36	1.31
26	BA	503	A	C8-N7	7.66	1.36	1.31
26	BA	1509	A	C8-N7	7.66	1.36	1.31
26	BA	1786	A	C8-N7	7.66	1.36	1.31
26	BA	2019	A	C8-N7	7.66	1.36	1.31
26	BA	412	A	C8-N7	7.65	1.36	1.31
26	BA	2682	A	C8-N7	7.65	1.36	1.31
1	AA	673	A	C8-N7	7.65	1.36	1.31
26	BA	1630	A	C8-N7	7.65	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	782	A	C8-N7	7.65	1.36	1.31
1	AA	1229	A	C8-N7	7.65	1.36	1.31
26	BA	918	A	C8-N7	7.65	1.36	1.31
26	BA	1858	A	C8-N7	7.65	1.36	1.31
1	AA	412	A	C8-N7	7.65	1.36	1.31
26	BA	2850	A	C8-N7	7.65	1.36	1.31
27	BB	115	A	C8-N7	7.65	1.36	1.31
26	BA	149	A	C8-N7	7.65	1.36	1.31
26	BA	165	A	C8-N7	7.65	1.36	1.31
26	BA	752	A	C8-N7	7.65	1.36	1.31
26	BA	1057	A	C8-N7	7.65	1.36	1.31
26	BA	2439	A	C8-N7	7.65	1.36	1.31
26	BA	980	A	C8-N7	7.65	1.36	1.31
26	BA	1597	A	C8-N7	7.65	1.36	1.31
26	BA	1705	A	C8-N7	7.65	1.36	1.31
1	AA	777	A	C8-N7	7.64	1.36	1.31
1	AA	1434	A	C8-N7	7.64	1.36	1.31
24	AX	21	A	C8-N7	7.64	1.36	1.31
26	BA	131	A	C8-N7	7.64	1.36	1.31
26	BA	219	A	C8-N7	7.64	1.36	1.31
26	BA	422	A	C8-N7	7.64	1.36	1.31
26	BA	739	A	C8-N7	7.64	1.36	1.31
26	BA	1815	A	C8-N7	7.64	1.36	1.31
1	AA	609	A	C8-N7	7.64	1.36	1.31
23	AW	26	A	C8-N7	7.64	1.36	1.31
26	BA	272	A	C8-N7	7.64	1.36	1.31
26	BA	382	A	C8-N7	7.64	1.36	1.31
26	BA	454	A	C8-N7	7.64	1.36	1.31
26	BA	990	A	C8-N7	7.64	1.36	1.31
26	BA	2872	A	C8-N7	7.64	1.36	1.31
1	AA	695	A	C8-N7	7.64	1.36	1.31
1	AA	1150	A	C8-N7	7.64	1.36	1.31
26	BA	104	A	C8-N7	7.64	1.36	1.31
26	BA	439	A	C8-N7	7.64	1.36	1.31
26	BA	1204	A	C8-N7	7.64	1.36	1.31
1	AA	602	A	C8-N7	7.64	1.36	1.31
1	AA	790	A	C8-N7	7.64	1.36	1.31
26	BA	504	A	C8-N7	7.64	1.36	1.31
26	BA	2266	A	C8-N7	7.64	1.36	1.31
26	BA	2792	A	C8-N7	7.64	1.36	1.31
26	BA	2882	A	C8-N7	7.64	1.36	1.31
1	AA	172	A	C8-N7	7.64	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1431	A	C8-N7	7.64	1.36	1.31
26	BA	927	A	C8-N7	7.64	1.36	1.31
26	BA	2154	A	C8-N7	7.64	1.36	1.31
26	BA	2542	A	C8-N7	7.64	1.36	1.31
1	AA	179	A	C8-N7	7.64	1.36	1.31
1	AA	274	A	C8-N7	7.64	1.36	1.31
1	AA	554	A	C8-N7	7.64	1.36	1.31
1	AA	694	A	C8-N7	7.64	1.36	1.31
1	AA	802	A	C8-N7	7.64	1.36	1.31
26	BA	144	A	C8-N7	7.64	1.36	1.31
26	BA	1275	A	C8-N7	7.64	1.36	1.31
26	BA	1744	A	C8-N7	7.64	1.36	1.31
26	BA	1987	A	C8-N7	7.64	1.36	1.31
26	BA	2170	A	C8-N7	7.64	1.36	1.31
26	BA	2298	A	C8-N7	7.64	1.36	1.31
1	AA	327	A	C8-N7	7.63	1.36	1.31
1	AA	344	A	C8-N7	7.63	1.36	1.31
1	AA	1227	A	C8-N7	7.63	1.36	1.31
25	AY	69	A	C8-N7	7.63	1.36	1.31
26	BA	111	A	C8-N7	7.63	1.36	1.31
26	BA	753	A	C8-N7	7.63	1.36	1.31
26	BA	861	A	C8-N7	7.63	1.36	1.31
26	BA	2736	A	C8-N7	7.63	1.36	1.31
26	BA	2809	A	C8-N7	7.63	1.36	1.31
1	AA	119	A	C8-N7	7.63	1.36	1.31
26	BA	866	A	C8-N7	7.63	1.36	1.31
26	BA	2740	A	C8-N7	7.63	1.36	1.31
1	AA	80	A	C8-N7	7.63	1.36	1.31
1	AA	747	A	C8-N7	7.63	1.36	1.31
1	AA	1269	A	C8-N7	7.63	1.36	1.31
25	AY	58	A	C8-N7	7.63	1.36	1.31
26	BA	788	A	C8-N7	7.63	1.36	1.31
26	BA	1214	A	C8-N7	7.63	1.36	1.31
26	BA	1366	A	C8-N7	7.63	1.36	1.31
26	BA	1580	A	C8-N7	7.63	1.36	1.31
26	BA	1789	A	C8-N7	7.63	1.36	1.31
1	AA	1519	A	C8-N7	7.63	1.36	1.31
26	BA	1593	A	C8-N7	7.63	1.36	1.31
26	BA	2632	A	C8-N7	7.63	1.36	1.31
1	AA	10	A	C8-N7	7.63	1.36	1.31
1	AA	676	A	C8-N7	7.63	1.36	1.31
1	AA	1413	A	C8-N7	7.63	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	310	A	C8-N7	7.63	1.36	1.31
26	BA	347	A	C8-N7	7.63	1.36	1.31
26	BA	896	A	C8-N7	7.63	1.36	1.31
26	BA	945	A	C8-N7	7.63	1.36	1.31
26	BA	1265	A	C8-N7	7.63	1.36	1.31
26	BA	1854	A	C8-N7	7.63	1.36	1.31
26	BA	2142	A	C8-N7	7.63	1.36	1.31
26	BA	2270	A	C8-N7	7.63	1.36	1.31
26	BA	2821	A	C8-N7	7.63	1.36	1.31
1	AA	675	A	C8-N7	7.63	1.36	1.31
1	AA	919	A	C8-N7	7.63	1.36	1.31
26	BA	802	A	C8-N7	7.63	1.36	1.31
26	BA	1272	A	C8-N7	7.63	1.36	1.31
26	BA	1307	A	C8-N7	7.63	1.36	1.31
26	BA	538	A	C8-N7	7.62	1.36	1.31
26	BA	1237	A	C8-N7	7.62	1.36	1.31
27	BB	39	A	C8-N7	7.62	1.36	1.31
1	AA	1446	A	C8-N7	7.62	1.36	1.31
26	BA	391	A	C8-N7	7.62	1.36	1.31
26	BA	428	A	C8-N7	7.62	1.36	1.31
26	BA	1548	A	C8-N7	7.62	1.36	1.31
26	BA	2899	A	C8-N7	7.62	1.36	1.31
1	AA	71	A	C8-N7	7.62	1.36	1.31
1	AA	120	A	C8-N7	7.62	1.36	1.31
1	AA	143	A	C8-N7	7.62	1.36	1.31
1	AA	199	A	C8-N7	7.62	1.36	1.31
1	AA	649	A	C8-N7	7.62	1.36	1.31
24	AX	23	A	C8-N7	7.62	1.36	1.31
24	AX	41	A	C8-N7	7.62	1.36	1.31
26	BA	244	A	C8-N7	7.62	1.36	1.31
26	BA	727	A	C8-N7	7.62	1.36	1.31
26	BA	734	A	C8-N7	7.62	1.36	1.31
26	BA	1321	A	C8-N7	7.62	1.36	1.31
26	BA	1634	A	C8-N7	7.62	1.36	1.31
26	BA	1885	A	C8-N7	7.62	1.36	1.31
26	BA	2670	A	C8-N7	7.62	1.36	1.31
1	AA	288	A	C8-N7	7.62	1.36	1.31
1	AA	1480	A	C8-N7	7.62	1.36	1.31
26	BA	1618	A	C8-N7	7.62	1.36	1.31
26	BA	1803	A	C8-N7	7.62	1.36	1.31
26	BA	2639	A	C8-N7	7.62	1.36	1.31
1	AA	495	A	C8-N7	7.62	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	560	A	C8-N7	7.62	1.36	1.31
1	AA	1082	A	C8-N7	7.62	1.36	1.31
26	BA	173	A	C8-N7	7.62	1.36	1.31
26	BA	241	A	C8-N7	7.62	1.36	1.31
26	BA	508	A	C8-N7	7.62	1.36	1.31
26	BA	602	A	C8-N7	7.62	1.36	1.31
26	BA	1067	A	C8-N7	7.62	1.36	1.31
26	BA	1144	A	C8-N7	7.62	1.36	1.31
26	BA	1552	A	C8-N7	7.62	1.36	1.31
26	BA	1654	A	C8-N7	7.62	1.36	1.31
26	BA	1877	A	C8-N7	7.62	1.36	1.31
26	BA	2199	A	C8-N7	7.62	1.36	1.31
26	BA	2448	A	C8-N7	7.62	1.36	1.31
1	AA	1447	A	C8-N7	7.62	1.36	1.31
26	BA	616	A	C8-N7	7.62	1.36	1.31
1	AA	787	A	C8-N7	7.62	1.36	1.31
22	AV	15	A	C8-N7	7.62	1.36	1.31
26	BA	125	A	C8-N7	7.62	1.36	1.31
26	BA	348	A	C8-N7	7.62	1.36	1.31
26	BA	374	A	C8-N7	7.62	1.36	1.31
26	BA	718	A	C8-N7	7.62	1.36	1.31
26	BA	1304	A	C8-N7	7.62	1.36	1.31
26	BA	1689	A	C8-N7	7.62	1.36	1.31
26	BA	1900	A	C8-N7	7.62	1.36	1.31
26	BA	1919	A	C8-N7	7.62	1.36	1.31
26	BA	2005	A	C8-N7	7.62	1.36	1.31
26	BA	2205	A	C8-N7	7.62	1.36	1.31
26	BA	2432	A	C8-N7	7.62	1.36	1.31
26	BA	2471	A	C8-N7	7.62	1.36	1.31
26	BA	2654	A	C8-N7	7.62	1.36	1.31
1	AA	393	A	C8-N7	7.61	1.36	1.31
1	AA	792	A	C8-N7	7.61	1.36	1.31
1	AA	1067	A	C8-N7	7.61	1.36	1.31
1	AA	1171	A	C8-N7	7.61	1.36	1.31
1	AA	1500	A	C8-N7	7.61	1.36	1.31
26	BA	654	A	C8-N7	7.61	1.36	1.31
26	BA	910	A	C8-N7	7.61	1.36	1.31
26	BA	1073	A	C8-N7	7.61	1.36	1.31
26	BA	1603	A	C8-N7	7.61	1.36	1.31
26	BA	1665	A	C8-N7	7.61	1.36	1.31
26	BA	2015	A	C8-N7	7.61	1.36	1.31
26	BA	2071	A	C8-N7	7.61	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2513	A	C8-N7	7.61	1.36	1.31
26	BA	2886	A	C8-N7	7.61	1.36	1.31
1	AA	1239	A	C8-N7	7.61	1.36	1.31
26	BA	352	A	C8-N7	7.61	1.36	1.31
26	BA	1010	A	C8-N7	7.61	1.36	1.31
26	BA	2412	A	C8-N7	7.61	1.36	1.31
1	AA	77	A	C8-N7	7.61	1.36	1.31
1	AA	435	A	C8-N7	7.61	1.36	1.31
1	AA	648	A	C8-N7	7.61	1.36	1.31
1	AA	969	A	C8-N7	7.61	1.36	1.31
1	AA	1254	A	C8-N7	7.61	1.36	1.31
1	AA	1531	A	C8-N7	7.61	1.36	1.31
24	AX	58	A	C8-N7	7.61	1.36	1.31
26	BA	233	A	C8-N7	7.61	1.36	1.31
26	BA	676	A	C8-N7	7.61	1.36	1.31
26	BA	1054	A	C8-N7	7.61	1.36	1.31
26	BA	1569	A	C8-N7	7.61	1.36	1.31
26	BA	1978	A	C8-N7	7.61	1.36	1.31
26	BA	2435	A	C8-N7	7.61	1.36	1.31
26	BA	2734	A	C8-N7	7.61	1.36	1.31
26	BA	282	A	C8-N7	7.61	1.36	1.31
26	BA	2566	A	C8-N7	7.61	1.36	1.31
1	AA	1288	A	C8-N7	7.61	1.36	1.31
26	BA	44	A	C8-N7	7.61	1.36	1.31
26	BA	217	A	C8-N7	7.61	1.36	1.31
26	BA	344	A	C8-N7	7.61	1.36	1.31
26	BA	460	A	C8-N7	7.61	1.36	1.31
26	BA	722	A	C8-N7	7.61	1.36	1.31
26	BA	1027	A	C8-N7	7.61	1.36	1.31
26	BA	1085	A	C8-N7	7.61	1.36	1.31
26	BA	1134	A	C8-N7	7.61	1.36	1.31
1	AA	101	A	C8-N7	7.61	1.36	1.31
1	AA	1408	A	C8-N7	7.61	1.36	1.31
26	BA	161	A	C8-N7	7.61	1.36	1.31
26	BA	1028	A	C8-N7	7.61	1.36	1.31
26	BA	2572	A	C8-N7	7.61	1.36	1.31
26	BA	2346	A	C8-N7	7.60	1.36	1.31
1	AA	704	A	C8-N7	7.60	1.36	1.31
1	AA	706	A	C8-N7	7.60	1.36	1.31
1	AA	1274	A	C8-N7	7.60	1.36	1.31
26	BA	324	A	C8-N7	7.60	1.36	1.31
26	BA	670	A	C8-N7	7.60	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	8	A	C8-N7	7.60	1.36	1.31
26	BA	478	A	C8-N7	7.60	1.36	1.31
26	BA	643	A	C8-N7	7.60	1.36	1.31
26	BA	1819	A	C8-N7	7.60	1.36	1.31
1	AA	430	A	C8-N7	7.60	1.36	1.31
1	AA	918	A	C8-N7	7.60	1.36	1.31
1	AA	1201	A	C8-N7	7.60	1.36	1.31
26	BA	322	A	C8-N7	7.60	1.36	1.31
26	BA	1453	A	C8-N7	7.60	1.36	1.31
26	BA	1746	A	C8-N7	7.60	1.36	1.31
26	BA	1927	A	C8-N7	7.60	1.36	1.31
26	BA	1952	A	C8-N7	7.60	1.36	1.31
26	BA	2278	A	C8-N7	7.60	1.36	1.31
26	BA	2727	A	C8-N7	7.60	1.36	1.31
27	BB	52	A	C8-N7	7.60	1.36	1.31
1	AA	374	A	C8-N7	7.60	1.36	1.31
1	AA	642	A	C8-N7	7.60	1.36	1.31
1	AA	1169	A	C8-N7	7.60	1.36	1.31
1	AA	1256	A	C8-N7	7.60	1.36	1.31
24	AX	9	A	C8-N7	7.60	1.36	1.31
26	BA	83	A	C8-N7	7.60	1.36	1.31
26	BA	270	A	C8-N7	7.60	1.36	1.31
26	BA	668	A	C8-N7	7.60	1.36	1.31
26	BA	1342	A	C8-N7	7.60	1.36	1.31
26	BA	2733	A	C8-N7	7.60	1.36	1.31
26	BA	2851	A	C8-N7	7.60	1.36	1.31
1	AA	1534	A	C8-N7	7.60	1.36	1.31
26	BA	156	A	C8-N7	7.60	1.36	1.31
1	AA	383	A	C8-N7	7.59	1.36	1.31
1	AA	461	A	C8-N7	7.59	1.36	1.31
1	AA	535	A	C8-N7	7.59	1.36	1.31
26	BA	84	A	C8-N7	7.59	1.36	1.31
26	BA	515	A	C8-N7	7.59	1.36	1.31
26	BA	1046	A	C8-N7	7.59	1.36	1.31
26	BA	1384	A	C8-N7	7.59	1.36	1.31
26	BA	1610	A	C8-N7	7.59	1.36	1.31
26	BA	2198	A	C8-N7	7.59	1.36	1.31
1	AA	460	A	C8-N7	7.59	1.36	1.31
22	AV	17	A	C8-N7	7.59	1.36	1.31
26	BA	362	A	C8-N7	7.59	1.36	1.31
26	BA	1932	A	C8-N7	7.59	1.36	1.31
26	BA	2037	A	C8-N7	7.59	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2541	A	C8-N7	7.59	1.36	1.31
1	AA	532	A	C8-N7	7.59	1.36	1.31
1	AA	746	A	C8-N7	7.59	1.36	1.31
1	AA	1465	A	C8-N7	7.59	1.36	1.31
25	AY	35	A	C8-N7	7.59	1.36	1.31
26	BA	199	A	C8-N7	7.59	1.36	1.31
26	BA	300	A	C8-N7	7.59	1.36	1.31
26	BA	404	A	C8-N7	7.59	1.36	1.31
26	BA	563	A	C8-N7	7.59	1.36	1.31
26	BA	1050	A	C8-N7	7.59	1.36	1.31
26	BA	1347	A	C8-N7	7.59	1.36	1.31
26	BA	1525	A	C8-N7	7.59	1.36	1.31
26	BA	1872	A	C8-N7	7.59	1.36	1.31
26	BA	2147	A	C8-N7	7.59	1.36	1.31
26	BA	2516	A	C8-N7	7.59	1.36	1.31
26	BA	2534	A	C8-N7	7.59	1.36	1.31
26	BA	2679	A	C8-N7	7.59	1.36	1.31
1	AA	236	A	C8-N7	7.59	1.36	1.31
1	AA	238	A	C8-N7	7.59	1.36	1.31
1	AA	389	A	C8-N7	7.59	1.36	1.31
1	AA	1012	A	C8-N7	7.59	1.36	1.31
1	AA	1360	A	C8-N7	7.59	1.36	1.31
26	BA	182	A	C8-N7	7.59	1.36	1.31
26	BA	221	A	C8-N7	7.59	1.36	1.31
26	BA	1142	A	C8-N7	7.59	1.36	1.31
26	BA	1890	A	C8-N7	7.59	1.36	1.31
1	AA	382	A	C8-N7	7.59	1.36	1.31
1	AA	553	A	C8-N7	7.59	1.36	1.31
25	AY	38	A	C8-N7	7.59	1.36	1.31
26	BA	309	A	C8-N7	7.59	1.36	1.31
26	BA	1084	A	C8-N7	7.59	1.36	1.31
26	BA	1508	A	C8-N7	7.59	1.36	1.31
26	BA	1616	A	C8-N7	7.59	1.36	1.31
26	BA	2883	A	C8-N7	7.59	1.36	1.31
1	AA	65	A	C8-N7	7.59	1.36	1.31
1	AA	279	A	C8-N7	7.59	1.36	1.31
1	AA	595	A	C8-N7	7.59	1.36	1.31
1	AA	1196	A	C8-N7	7.59	1.36	1.31
23	AW	14	A	C8-N7	7.59	1.36	1.31
23	AW	21	A	C8-N7	7.59	1.36	1.31
24	AX	26	A	C8-N7	7.59	1.36	1.31
26	BA	64	A	C8-N7	7.59	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	613	A	C8-N7	7.59	1.36	1.31
26	BA	764	A	C8-N7	7.59	1.36	1.31
26	BA	781	A	C8-N7	7.59	1.36	1.31
26	BA	1711	A	C8-N7	7.59	1.36	1.31
26	BA	1735	A	C8-N7	7.59	1.36	1.31
26	BA	1780	A	C8-N7	7.59	1.36	1.31
26	BA	1808	A	C8-N7	7.59	1.36	1.31
26	BA	2119	A	C8-N7	7.59	1.36	1.31
26	BA	2176	A	C8-N7	7.59	1.36	1.31
1	AA	583	A	C8-N7	7.58	1.36	1.31
25	AY	14	A	C8-N7	7.58	1.36	1.31
26	BA	608	A	C8-N7	7.58	1.36	1.31
26	BA	1579	A	C8-N7	7.58	1.36	1.31
26	BA	1916	A	C8-N7	7.58	1.36	1.31
1	AA	1285	A	C8-N7	7.58	1.36	1.31
25	AY	9	A	C8-N7	7.58	1.36	1.31
26	BA	631	A	C8-N7	7.58	1.36	1.31
26	BA	821	A	C8-N7	7.58	1.36	1.31
26	BA	1165	A	C8-N7	7.58	1.36	1.31
1	AA	253	A	C8-N7	7.58	1.36	1.31
1	AA	1250	A	C8-N7	7.58	1.36	1.31
1	AA	1503	A	C8-N7	7.58	1.36	1.31
26	BA	222	A	C8-N7	7.58	1.36	1.31
26	BA	332	A	C8-N7	7.58	1.36	1.31
26	BA	1246	A	C8-N7	7.58	1.36	1.31
26	BA	1268	A	C8-N7	7.58	1.36	1.31
26	BA	1503	A	C8-N7	7.58	1.36	1.31
27	BB	94	A	C8-N7	7.58	1.36	1.31
26	BA	126	A	C8-N7	7.58	1.36	1.31
26	BA	575	A	C8-N7	7.58	1.36	1.31
26	BA	899	A	C8-N7	7.58	1.36	1.31
26	BA	1551	A	C8-N7	7.58	1.36	1.31
26	BA	1668	A	C8-N7	7.58	1.36	1.31
26	BA	2309	A	C8-N7	7.58	1.36	1.31
26	BA	2476	A	C8-N7	7.58	1.36	1.31
1	AA	441	A	C8-N7	7.58	1.36	1.31
1	AA	630	A	C8-N7	7.58	1.36	1.31
1	AA	781	A	C8-N7	7.58	1.36	1.31
1	AA	784	A	C8-N7	7.58	1.36	1.31
26	BA	547	A	C8-N7	7.58	1.36	1.31
26	BA	1000	A	C8-N7	7.58	1.36	1.31
26	BA	1609	A	C8-N7	7.58	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1848	A	C8-N7	7.58	1.36	1.31
26	BA	2453	A	C8-N7	7.58	1.36	1.31
26	BA	2711	A	C8-N7	7.58	1.36	1.31
26	BA	1089	A	C8-N7	7.58	1.36	1.31
26	BA	1505	A	C8-N7	7.58	1.36	1.31
26	BA	2590	A	C8-N7	7.58	1.36	1.31
1	AA	468	A	C8-N7	7.58	1.36	1.31
1	AA	996	A	C8-N7	7.58	1.36	1.31
26	BA	345	A	C8-N7	7.58	1.36	1.31
26	BA	1069	A	C8-N7	7.58	1.36	1.31
26	BA	1129	A	C8-N7	7.58	1.36	1.31
26	BA	1392	A	C8-N7	7.58	1.36	1.31
26	BA	2503	A	C8-N7	7.58	1.36	1.31
1	AA	59	A	C8-N7	7.57	1.36	1.31
1	AA	596	A	C8-N7	7.57	1.36	1.31
1	AA	1042	A	C8-N7	7.57	1.36	1.31
1	AA	1180	A	C8-N7	7.57	1.36	1.31
1	AA	1204	A	C8-N7	7.57	1.36	1.31
23	AW	31	A	C8-N7	7.57	1.36	1.31
26	BA	1353	A	C8-N7	7.57	1.36	1.31
26	BA	1672	A	C8-N7	7.57	1.36	1.31
1	AA	250	A	C8-N7	7.57	1.36	1.31
1	AA	349	A	C8-N7	7.57	1.36	1.31
1	AA	663	A	C8-N7	7.57	1.36	1.31
1	AA	768	A	C8-N7	7.57	1.36	1.31
27	BB	99	A	C8-N7	7.57	1.36	1.31
1	AA	629	A	C8-N7	7.57	1.36	1.31
1	AA	687	A	C8-N7	7.57	1.36	1.31
1	AA	964	A	C8-N7	7.57	1.36	1.31
26	BA	279	A	C8-N7	7.57	1.36	1.31
26	BA	749	A	C8-N7	7.57	1.36	1.31
26	BA	900	A	C8-N7	7.57	1.36	1.31
26	BA	1496	A	C8-N7	7.57	1.36	1.31
26	BA	2660	A	C8-N7	7.57	1.36	1.31
1	AA	325	A	C8-N7	7.57	1.36	1.31
1	AA	336	A	C8-N7	7.57	1.36	1.31
26	BA	5	A	C8-N7	7.57	1.36	1.31
26	BA	91	A	C8-N7	7.57	1.36	1.31
1	AA	161	A	C8-N7	7.57	1.36	1.31
1	AA	167	A	C8-N7	7.57	1.36	1.31
1	AA	364	A	C8-N7	7.57	1.36	1.31
1	AA	547	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	1055	A	C8-N7	7.57	1.36	1.31
1	AA	1179	A	C8-N7	7.57	1.36	1.31
26	BA	715	A	C8-N7	7.57	1.36	1.31
26	BA	1077	A	C8-N7	7.57	1.36	1.31
26	BA	2227	A	C8-N7	7.57	1.36	1.31
1	AA	1145	A	C8-N7	7.57	1.36	1.31
1	AA	1340	A	C8-N7	7.57	1.36	1.31
26	BA	742	A	C8-N7	7.57	1.36	1.31
26	BA	988	A	C8-N7	7.57	1.36	1.31
26	BA	1373	A	C8-N7	7.57	1.36	1.31
26	BA	2406	A	C8-N7	7.57	1.36	1.31
26	BA	2810	A	C8-N7	7.57	1.36	1.31
1	AA	228	A	C8-N7	7.56	1.36	1.31
26	BA	1127	A	C8-N7	7.56	1.36	1.31
1	AA	28	A	C8-N7	7.56	1.36	1.31
1	AA	712	A	C8-N7	7.56	1.36	1.31
1	AA	780	A	C8-N7	7.56	1.36	1.31
1	AA	1456	A	C8-N7	7.56	1.36	1.31
23	AW	69	A	C8-N7	7.56	1.36	1.31
26	BA	160	A	C8-N7	7.56	1.36	1.31
26	BA	501	A	C8-N7	7.56	1.36	1.31
26	BA	1773	A	C8-N7	7.56	1.36	1.31
26	BA	2340	A	C8-N7	7.56	1.36	1.31
26	BA	2377	A	C8-N7	7.56	1.36	1.31
26	BA	2577	A	C8-N7	7.56	1.36	1.31
27	BB	66	A	C8-N7	7.56	1.36	1.31
27	BB	119	A	C8-N7	7.56	1.36	1.31
1	AA	81	A	C8-N7	7.56	1.36	1.31
1	AA	174	A	C8-N7	7.56	1.36	1.31
1	AA	878	A	C8-N7	7.56	1.36	1.31
26	BA	789	A	C8-N7	7.56	1.36	1.31
26	BA	2411	A	C8-N7	7.56	1.36	1.31
1	AA	819	A	C8-N7	7.56	1.36	1.31
1	AA	1092	A	C8-N7	7.56	1.36	1.31
1	AA	1492	A	C8-N7	7.56	1.36	1.31
23	AW	66	A	C8-N7	7.56	1.36	1.31
26	BA	735	A	C8-N7	7.56	1.36	1.31
26	BA	1367	A	C8-N7	7.56	1.36	1.31
26	BA	1655	A	C8-N7	7.56	1.36	1.31
26	BA	2212	A	C8-N7	7.56	1.36	1.31
26	BA	2900	A	C8-N7	7.56	1.36	1.31
1	AA	197	A	C8-N7	7.56	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1225	A	C8-N7	7.56	1.36	1.31
1	AA	1287	A	C8-N7	7.56	1.36	1.31
26	BA	265	A	C8-N7	7.56	1.36	1.31
26	BA	892	A	C8-N7	7.56	1.36	1.31
26	BA	1009	A	C8-N7	7.56	1.36	1.31
26	BA	1470	A	C8-N7	7.56	1.36	1.31
26	BA	2781	A	C8-N7	7.56	1.36	1.31
26	BA	2860	A	C8-N7	7.56	1.36	1.31
1	AA	2	A	C8-N7	7.56	1.36	1.31
1	AA	181	A	C8-N7	7.56	1.36	1.31
1	AA	974	A	C8-N7	7.56	1.36	1.31
1	AA	975	A	C8-N7	7.56	1.36	1.31
1	AA	1197	A	C8-N7	7.56	1.36	1.31
25	AY	21	A	C8-N7	7.56	1.36	1.31
26	BA	118	A	C8-N7	7.56	1.36	1.31
26	BA	483	A	C8-N7	7.56	1.36	1.31
26	BA	1608	A	C8-N7	7.56	1.36	1.31
26	BA	2726	A	C8-N7	7.56	1.36	1.31
1	AA	189	A	C8-N7	7.55	1.36	1.31
1	AA	860	A	C8-N7	7.55	1.36	1.31
1	AA	1046	A	C8-N7	7.55	1.36	1.31
1	AA	1110	A	C8-N7	7.55	1.36	1.31
1	AA	1437	A	C8-N7	7.55	1.36	1.31
26	BA	1502	A	C8-N7	7.55	1.36	1.31
26	BA	1528	A	C8-N7	7.55	1.36	1.31
26	BA	1586	A	C8-N7	7.55	1.36	1.31
26	BA	1749	A	C8-N7	7.55	1.36	1.31
26	BA	2059	A	C8-N7	7.55	1.36	1.31
26	BA	2564	A	C8-N7	7.55	1.36	1.31
26	BA	2757	A	C8-N7	7.55	1.36	1.31
1	AA	573	A	C8-N7	7.55	1.36	1.31
1	AA	1146	A	C8-N7	7.55	1.36	1.31
26	BA	13	A	C8-N7	7.55	1.36	1.31
26	BA	947	A	C8-N7	7.55	1.36	1.31
26	BA	1504	A	C8-N7	7.55	1.36	1.31
26	BA	1717	A	C8-N7	7.55	1.36	1.31
26	BA	1871	A	C8-N7	7.55	1.36	1.31
26	BA	1889	A	C8-N7	7.55	1.36	1.31
26	BA	2434	A	C8-N7	7.55	1.36	1.31
1	AA	3	A	C8-N7	7.55	1.36	1.31
1	AA	715	A	C8-N7	7.55	1.36	1.31
26	BA	218	A	C8-N7	7.55	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1020	A	C8-N7	7.55	1.36	1.31
26	BA	1591	A	C8-N7	7.55	1.36	1.31
26	BA	2042	A	C8-N7	7.55	1.36	1.31
26	BA	2814	A	C8-N7	7.55	1.36	1.31
1	AA	16	A	C8-N7	7.55	1.36	1.31
1	AA	448	A	C8-N7	7.55	1.36	1.31
1	AA	1271	A	C8-N7	7.55	1.36	1.31
26	BA	42	A	C8-N7	7.55	1.36	1.31
26	BA	677	A	C8-N7	7.55	1.36	1.31
1	AA	539	A	C8-N7	7.55	1.36	1.31
1	AA	702	A	C8-N7	7.55	1.36	1.31
1	AA	759	A	C8-N7	7.55	1.36	1.31
1	AA	1016	A	C8-N7	7.55	1.36	1.31
26	BA	661	A	C8-N7	7.55	1.36	1.31
26	BA	1086	A	C8-N7	7.55	1.36	1.31
26	BA	1103	A	C8-N7	7.55	1.36	1.31
26	BA	1739	A	C8-N7	7.55	1.36	1.31
26	BA	2813	A	C8-N7	7.55	1.36	1.31
1	AA	98	A	C8-N7	7.54	1.36	1.31
1	AA	635	A	C8-N7	7.54	1.36	1.31
1	AA	696	A	C8-N7	7.54	1.36	1.31
1	AA	767	A	C8-N7	7.54	1.36	1.31
26	BA	626	A	C8-N7	7.54	1.36	1.31
26	BA	730	A	C8-N7	7.54	1.36	1.31
26	BA	1322	A	C8-N7	7.54	1.36	1.31
1	AA	53	A	C8-N7	7.54	1.36	1.31
1	AA	55	A	C8-N7	7.54	1.36	1.31
1	AA	572	A	C8-N7	7.54	1.36	1.31
1	AA	1349	A	C8-N7	7.54	1.36	1.31
26	BA	223	A	C8-N7	7.54	1.36	1.31
26	BA	1048	A	C8-N7	7.54	1.36	1.31
26	BA	1431	A	C8-N7	7.54	1.36	1.31
26	BA	1722	A	C8-N7	7.54	1.36	1.31
26	BA	2461	A	C8-N7	7.54	1.36	1.31
26	BA	2482	A	C8-N7	7.54	1.36	1.31
26	BA	2587	A	C8-N7	7.54	1.36	1.31
27	BB	15	A	C8-N7	7.54	1.36	1.31
1	AA	600	A	C8-N7	7.54	1.36	1.31
1	AA	1213	A	C8-N7	7.54	1.36	1.31
1	AA	1513	A	C8-N7	7.54	1.36	1.31
26	BA	53	A	C8-N7	7.54	1.36	1.31
26	BA	1247	A	C8-N7	7.54	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2117	A	C8-N7	7.54	1.36	1.31
26	BA	627	A	C8-N7	7.54	1.36	1.31
26	BA	996	A	C8-N7	7.54	1.36	1.31
26	BA	2169	A	C8-N7	7.54	1.36	1.31
1	AA	19	A	C8-N7	7.54	1.36	1.31
1	AA	958	A	C8-N7	7.54	1.36	1.31
1	AA	1280	A	C8-N7	7.54	1.36	1.31
26	BA	603	A	C8-N7	7.54	1.36	1.31
26	BA	693	A	C8-N7	7.54	1.36	1.31
26	BA	943	A	C8-N7	7.54	1.36	1.31
26	BA	1032	A	C8-N7	7.54	1.36	1.31
26	BA	1632	A	C8-N7	7.54	1.36	1.31
26	BA	1821	A	C8-N7	7.54	1.36	1.31
26	BA	2097	A	C8-N7	7.54	1.36	1.31
27	BB	73	A	C8-N7	7.54	1.36	1.31
1	AA	892	A	C8-N7	7.54	1.36	1.31
1	AA	1163	A	C8-N7	7.54	1.36	1.31
26	BA	1274	A	C8-N7	7.54	1.36	1.31
26	BA	2614	A	C8-N7	7.54	1.36	1.31
1	AA	7	A	C8-N7	7.54	1.36	1.31
1	AA	520	A	C8-N7	7.54	1.36	1.31
1	AA	728	A	C8-N7	7.54	1.36	1.31
1	AA	1346	A	C8-N7	7.54	1.36	1.31
24	AX	3	A	C8-N7	7.54	1.36	1.31
26	BA	311	A	C8-N7	7.54	1.36	1.31
26	BA	721	A	C8-N7	7.54	1.36	1.31
26	BA	1596	A	C8-N7	7.54	1.36	1.31
26	BA	1677	A	C8-N7	7.54	1.36	1.31
26	BA	1678	A	C8-N7	7.54	1.36	1.31
26	BA	1805	A	C8-N7	7.54	1.36	1.31
1	AA	51	A	C8-N7	7.53	1.36	1.31
1	AA	487	A	C8-N7	7.53	1.36	1.31
1	AA	794	A	C8-N7	7.53	1.36	1.31
1	AA	1111	A	C8-N7	7.53	1.36	1.31
26	BA	1544	A	C8-N7	7.53	1.36	1.31
26	BA	2378	A	C8-N7	7.53	1.36	1.31
25	AY	41	A	C8-N7	7.53	1.36	1.31
26	BA	195	A	C8-N7	7.53	1.36	1.31
26	BA	2284	A	C8-N7	7.53	1.36	1.31
27	BB	101	A	C8-N7	7.53	1.36	1.31
27	BB	109	A	C8-N7	7.53	1.36	1.31
23	AW	59	A	C8-N7	7.53	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	14	A	C8-N7	7.53	1.36	1.31
26	BA	203	A	C8-N7	7.53	1.36	1.31
26	BA	582	A	C8-N7	7.53	1.36	1.31
26	BA	845	A	C8-N7	7.53	1.36	1.31
26	BA	1039	A	C8-N7	7.53	1.36	1.31
26	BA	1090	A	C8-N7	7.53	1.36	1.31
26	BA	1205	A	C8-N7	7.53	1.36	1.31
1	AA	466	A	C8-N7	7.53	1.36	1.31
23	AW	41	A	C8-N7	7.53	1.36	1.31
26	BA	14	A	C8-N7	7.53	1.36	1.31
26	BA	2758	A	C8-N7	7.53	1.36	1.31
1	AA	482	A	C8-N7	7.53	1.36	1.31
1	AA	816	A	C8-N7	7.53	1.36	1.31
1	AA	1080	A	C8-N7	7.53	1.36	1.31
26	BA	833	A	C8-N7	7.53	1.36	1.31
26	BA	1420	A	C8-N7	7.53	1.36	1.31
26	BA	2518	A	C8-N7	7.53	1.36	1.31
27	BB	29	A	C8-N7	7.53	1.36	1.31
27	BB	108	A	C8-N7	7.53	1.36	1.31
1	AA	478	A	C8-N7	7.53	1.36	1.31
1	AA	1014	A	C8-N7	7.53	1.36	1.31
1	AA	1101	A	C8-N7	7.53	1.36	1.31
1	AA	1324	A	C8-N7	7.53	1.36	1.31
1	AA	1499	A	C8-N7	7.53	1.36	1.31
26	BA	152	A	C8-N7	7.53	1.36	1.31
26	BA	213	A	C8-N7	7.53	1.36	1.31
26	BA	699	A	C8-N7	7.53	1.36	1.31
26	BA	2183	A	C8-N7	7.53	1.36	1.31
1	AA	60	A	C8-N7	7.52	1.36	1.31
1	AA	155	A	C8-N7	7.52	1.36	1.31
1	AA	523	A	C8-N7	7.52	1.36	1.31
1	AA	1251	A	C8-N7	7.52	1.36	1.31
1	AA	1332	A	C8-N7	7.52	1.36	1.31
25	AY	6	A	C8-N7	7.52	1.36	1.31
26	BA	299	A	C8-N7	7.52	1.36	1.31
26	BA	979	A	C8-N7	7.52	1.36	1.31
26	BA	1759	A	C8-N7	7.52	1.36	1.31
27	BB	58	A	C8-N7	7.52	1.36	1.31
1	AA	465	A	C8-N7	7.52	1.36	1.31
1	AA	1362	A	C8-N7	7.52	1.36	1.31
1	AA	1377	A	C8-N7	7.52	1.36	1.31
26	BA	432	A	C8-N7	7.52	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	761	A	C8-N7	7.52	1.36	1.31
26	BA	2163	A	C8-N7	7.52	1.36	1.31
1	AA	906	A	C8-N7	7.52	1.36	1.31
26	BA	1532	A	C8-N7	7.52	1.36	1.31
26	BA	2879	A	C8-N7	7.52	1.36	1.31
1	AA	32	A	C8-N7	7.52	1.36	1.31
1	AA	149	A	C8-N7	7.52	1.36	1.31
1	AA	1036	A	C8-N7	7.52	1.36	1.31
26	BA	514	A	C8-N7	7.52	1.36	1.31
26	BA	599	A	C8-N7	7.52	1.36	1.31
26	BA	750	A	C8-N7	7.52	1.36	1.31
26	BA	1133	A	C8-N7	7.52	1.36	1.31
26	BA	1285	A	C8-N7	7.52	1.36	1.31
26	BA	1327	A	C8-N7	7.52	1.36	1.31
26	BA	1938	A	C8-N7	7.52	1.36	1.31
1	AA	262	A	C8-N7	7.52	1.36	1.31
1	AA	579	A	C8-N7	7.52	1.36	1.31
1	AA	864	A	C8-N7	7.52	1.36	1.31
23	AW	58	A	C8-N7	7.52	1.36	1.31
26	BA	73	A	C8-N7	7.52	1.36	1.31
26	BA	522	A	C8-N7	7.52	1.36	1.31
26	BA	917	A	C8-N7	7.52	1.36	1.31
26	BA	1626	A	C8-N7	7.52	1.36	1.31
26	BA	2247	A	C8-N7	7.52	1.36	1.31
26	BA	2893	A	C8-N7	7.52	1.36	1.31
1	AA	1441	A	C8-N7	7.52	1.36	1.31
26	BA	231	A	C8-N7	7.52	1.36	1.31
26	BA	1912	A	C8-N7	7.52	1.36	1.31
26	BA	2126	A	C8-N7	7.52	1.36	1.31
26	BA	2211	A	C8-N7	7.52	1.36	1.31
1	AA	353	A	C8-N7	7.51	1.36	1.31
1	AA	1093	A	C8-N7	7.51	1.36	1.31
1	AA	1105	A	C8-N7	7.51	1.36	1.31
1	AA	1375	A	C8-N7	7.51	1.36	1.31
26	BA	262	A	C8-N7	7.51	1.36	1.31
26	BA	294	A	C8-N7	7.51	1.36	1.31
26	BA	936	A	C8-N7	7.51	1.36	1.31
26	BA	1096	A	C8-N7	7.51	1.36	1.31
26	BA	1637	A	C8-N7	7.51	1.36	1.31
26	BA	1847	A	C8-N7	7.51	1.36	1.31
26	BA	2634	A	C8-N7	7.51	1.36	1.31
26	BA	2721	A	C8-N7	7.51	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2602	A	C8-N7	7.51	1.36	1.31
1	AA	356	A	C8-N7	7.51	1.36	1.31
24	AX	76	A	C8-N7	7.51	1.36	1.31
26	BA	256	A	C8-N7	7.51	1.36	1.31
26	BA	614	A	C8-N7	7.51	1.36	1.31
26	BA	716	A	C8-N7	7.51	1.36	1.31
26	BA	975	A	C8-N7	7.51	1.36	1.31
26	BA	1126	A	C8-N7	7.51	1.36	1.31
26	BA	1966	A	C8-N7	7.51	1.36	1.31
26	BA	1998	A	C8-N7	7.51	1.36	1.31
26	BA	2184	A	C8-N7	7.51	1.36	1.31
1	AA	116	A	C8-N7	7.51	1.36	1.31
1	AA	716	A	C8-N7	7.51	1.36	1.31
1	AA	815	A	C8-N7	7.51	1.36	1.31
1	AA	1257	A	C8-N7	7.51	1.36	1.31
1	AA	1433	A	C8-N7	7.51	1.36	1.31
26	BA	482	A	C8-N7	7.51	1.36	1.31
26	BA	928	A	C8-N7	7.51	1.36	1.31
26	BA	941	A	C8-N7	7.51	1.36	1.31
26	BA	1936	A	C8-N7	7.51	1.36	1.31
26	BA	1981	A	C8-N7	7.51	1.36	1.31
1	AA	498	A	C8-N7	7.51	1.36	1.31
1	AA	574	A	C8-N7	7.51	1.36	1.31
26	BA	181	A	C8-N7	7.51	1.36	1.31
26	BA	1262	A	C8-N7	7.51	1.36	1.31
26	BA	1383	A	C8-N7	7.51	1.36	1.31
26	BA	1403	A	C8-N7	7.51	1.36	1.31
26	BA	1679	A	C8-N7	7.51	1.36	1.31
26	BA	2060	A	C8-N7	7.51	1.36	1.31
1	AA	130	A	C8-N7	7.51	1.36	1.31
1	AA	743	A	C8-N7	7.51	1.36	1.31
1	AA	831	A	C8-N7	7.51	1.36	1.31
1	AA	949	A	C8-N7	7.51	1.36	1.31
26	BA	227	A	C8-N7	7.51	1.36	1.31
26	BA	804	A	C8-N7	7.51	1.36	1.31
27	BB	50	A	C8-N7	7.51	1.36	1.31
26	BA	101	A	C8-N7	7.50	1.36	1.31
1	AA	845	A	C8-N7	7.50	1.36	1.31
22	AV	21	A	C8-N7	7.50	1.36	1.31
1	AA	338	A	C8-N7	7.50	1.36	1.31
1	AA	607	A	C8-N7	7.50	1.36	1.31
1	AA	1130	A	C8-N7	7.50	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	191	A	C8-N7	7.50	1.36	1.31
26	BA	449	A	C8-N7	7.50	1.36	1.31
26	BA	666	A	C8-N7	7.50	1.36	1.31
26	BA	792	A	C8-N7	7.50	1.36	1.31
26	BA	829	A	C8-N7	7.50	1.36	1.31
26	BA	1008	A	C8-N7	7.50	1.36	1.31
26	BA	1269	A	C8-N7	7.50	1.36	1.31
26	BA	1713	A	C8-N7	7.50	1.36	1.31
26	BA	2088	A	C8-N7	7.50	1.36	1.31
1	AA	451	A	C8-N7	7.50	1.36	1.31
1	AA	1319	A	C8-N7	7.50	1.36	1.31
26	BA	176	A	C8-N7	7.50	1.36	1.31
26	BA	2336	A	C8-N7	7.50	1.36	1.31
1	AA	192	A	C8-N7	7.50	1.36	1.31
1	AA	807	A	C8-N7	7.50	1.36	1.31
1	AA	937	A	C8-N7	7.50	1.36	1.31
1	AA	1081	A	C8-N7	7.50	1.36	1.31
1	AA	1236	A	C8-N7	7.50	1.36	1.31
26	BA	1021	A	C8-N7	7.50	1.36	1.31
26	BA	1284	A	C8-N7	7.50	1.36	1.31
26	BA	1433	A	C8-N7	7.50	1.36	1.31
26	BA	2665	A	C8-N7	7.50	1.36	1.31
27	BB	57	A	C8-N7	7.50	1.36	1.31
1	AA	1394	A	C8-N7	7.50	1.36	1.31
1	AA	1430	A	C8-N7	7.50	1.36	1.31
26	BA	1287	A	C8-N7	7.50	1.36	1.31
26	BA	2054	A	C8-N7	7.50	1.36	1.31
1	AA	432	A	C8-N7	7.49	1.36	1.31
1	AA	1306	A	C8-N7	7.49	1.36	1.31
26	BA	1143	A	C8-N7	7.49	1.36	1.31
26	BA	1490	A	C8-N7	7.49	1.36	1.31
26	BA	2837	A	C8-N7	7.49	1.36	1.31
1	AA	363	A	C8-N7	7.49	1.36	1.31
22	AV	20	A	C8-N7	7.49	1.36	1.31
25	AY	26	A	C8-N7	7.49	1.36	1.31
26	BA	216	A	C8-N7	7.49	1.36	1.31
26	BA	1080	A	C8-N7	7.49	1.36	1.31
26	BA	2013	A	C8-N7	7.49	1.36	1.31
26	BA	2333	A	C8-N7	7.49	1.36	1.31
26	BA	2700	A	C8-N7	7.49	1.36	1.31
1	AA	306	A	C8-N7	7.49	1.36	1.31
1	AA	959	A	C8-N7	7.49	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1261	A	C8-N7	7.49	1.36	1.31
1	AA	1396	A	C8-N7	7.49	1.36	1.31
1	AA	1476	A	C8-N7	7.49	1.36	1.31
1	AA	1507	A	C8-N7	7.49	1.36	1.31
26	BA	443	A	C8-N7	7.49	1.36	1.31
26	BA	477	A	C8-N7	7.49	1.36	1.31
26	BA	689	A	C8-N7	7.49	1.36	1.31
26	BA	925	A	C8-N7	7.49	1.36	1.31
26	BA	1156	A	C8-N7	7.49	1.36	1.31
26	BA	1802	A	C8-N7	7.49	1.36	1.31
26	BA	2158	A	C8-N7	7.49	1.36	1.31
1	AA	1216	A	C8-N7	7.49	1.36	1.31
26	BA	507	A	C8-N7	7.49	1.36	1.31
26	BA	1754	A	C8-N7	7.49	1.36	1.31
26	BA	1928	A	C8-N7	7.49	1.36	1.31
27	BB	53	A	C8-N7	7.49	1.36	1.31
26	BA	423	A	C8-N7	7.49	1.36	1.31
26	BA	541	A	C8-N7	7.49	1.36	1.31
26	BA	609	A	C8-N7	7.49	1.36	1.31
26	BA	1698	A	C8-N7	7.49	1.36	1.31
26	BA	2497	A	C8-N7	7.49	1.36	1.31
26	BA	2565	A	C8-N7	7.49	1.36	1.31
26	BA	103	A	C8-N7	7.48	1.36	1.31
26	BA	1469	A	C8-N7	7.48	1.36	1.31
1	AA	50	A	C8-N7	7.48	1.36	1.31
1	AA	263	A	C8-N7	7.48	1.36	1.31
1	AA	559	A	C8-N7	7.48	1.36	1.31
26	BA	751	A	C8-N7	7.48	1.36	1.31
26	BA	1571	A	C8-N7	7.48	1.36	1.31
26	BA	2094	A	C8-N7	7.48	1.36	1.31
26	BA	2268	A	C8-N7	7.48	1.36	1.31
26	BA	2376	A	C8-N7	7.48	1.36	1.31
26	BA	2873	A	C8-N7	7.48	1.36	1.31
1	AA	33	A	C8-N7	7.48	1.36	1.31
1	AA	298	A	C8-N7	7.48	1.36	1.31
1	AA	496	A	C8-N7	7.48	1.36	1.31
1	AA	1191	A	C8-N7	7.48	1.36	1.31
26	BA	74	A	C8-N7	7.48	1.36	1.31
26	BA	94	A	C8-N7	7.48	1.36	1.31
26	BA	1264	A	C8-N7	7.48	1.36	1.31
26	BA	1354	A	C8-N7	7.48	1.36	1.31
26	BA	1676	A	C8-N7	7.48	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	38	A	C8-N7	7.48	1.36	1.31
26	BA	1088	A	C8-N7	7.48	1.36	1.31
26	BA	2725	A	C8-N7	7.48	1.36	1.31
1	AA	373	A	C8-N7	7.48	1.36	1.31
1	AA	1176	A	C8-N7	7.48	1.36	1.31
26	BA	19	A	C8-N7	7.48	1.36	1.31
26	BA	172	A	C8-N7	7.48	1.36	1.31
26	BA	368	A	C8-N7	7.48	1.36	1.31
26	BA	1650	A	C8-N7	7.48	1.36	1.31
26	BA	2020	A	C8-N7	7.48	1.36	1.31
26	BA	2062	A	C8-N7	7.48	1.36	1.31
26	BA	2273	A	C8-N7	7.48	1.36	1.31
26	BA	2317	A	C8-N7	7.48	1.36	1.31
26	BA	2657	A	C8-N7	7.48	1.36	1.31
1	AA	938	A	C8-N7	7.47	1.36	1.31
24	AX	24	A	C8-N7	7.47	1.36	1.31
26	BA	71	A	C8-N7	7.47	1.36	1.31
26	BA	505	A	C8-N7	7.47	1.36	1.31
26	BA	1226	A	C8-N7	7.47	1.36	1.31
26	BA	1494	A	C8-N7	7.47	1.36	1.31
26	BA	453	A	C8-N7	7.47	1.36	1.31
26	BA	1169	A	C8-N7	7.47	1.36	1.31
26	BA	2705	A	C8-N7	7.47	1.36	1.31
26	BA	2820	A	C8-N7	7.47	1.36	1.31
26	BA	1253	A	C8-N7	7.47	1.36	1.31
1	AA	935	A	C8-N7	7.47	1.36	1.31
26	BA	6	A	C8-N7	7.47	1.36	1.31
26	BA	972	A	C8-N7	7.47	1.36	1.31
26	BA	1070	A	C8-N7	7.47	1.36	1.31
26	BA	2433	A	C8-N7	7.47	1.36	1.31
26	BA	2750	A	C8-N7	7.47	1.36	1.31
26	BA	2799	A	C8-N7	7.47	1.36	1.31
26	BA	2392	A	C8-N7	7.47	1.36	1.31
26	BA	2468	A	C8-N7	7.47	1.36	1.31
26	BA	402	A	C8-N7	7.47	1.36	1.31
26	BA	2281	A	C8-N7	7.47	1.36	1.31
1	AA	1004	A	C8-N7	7.46	1.36	1.31
1	AA	1021	A	C8-N7	7.46	1.36	1.31
26	BA	1572	A	C8-N7	7.46	1.36	1.31
26	BA	1640	A	C8-N7	7.46	1.36	1.31
26	BA	849	A	C8-N7	7.46	1.36	1.31
26	BA	1151	A	C8-N7	7.46	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	977	A	C8-N7	7.46	1.36	1.31
26	BA	632	A	C8-N7	7.46	1.36	1.31
26	BA	2369	A	C8-N7	7.46	1.36	1.31
1	AA	414	A	C8-N7	7.46	1.36	1.31
1	AA	718	A	C8-N7	7.46	1.36	1.31
1	AA	1502	A	C8-N7	7.46	1.36	1.31
26	BA	492	A	C8-N7	7.46	1.36	1.31
26	BA	782	A	C8-N7	7.46	1.36	1.31
26	BA	2327	A	C8-N7	7.46	1.36	1.31
26	BA	2352	A	C8-N7	7.46	1.36	1.31
1	AA	321	A	C8-N7	7.46	1.36	1.31
1	AA	1508	A	C8-N7	7.46	1.36	1.31
26	BA	528	A	C8-N7	7.46	1.36	1.31
26	BA	556	A	C8-N7	7.46	1.36	1.31
26	BA	1434	A	C8-N7	7.46	1.36	1.31
26	BA	2191	A	C8-N7	7.46	1.36	1.31
1	AA	1518	A	C8-N7	7.46	1.36	1.31
26	BA	1189	A	C8-N7	7.46	1.36	1.31
26	BA	1495	A	C8-N7	7.46	1.36	1.31
26	BA	1977	A	C8-N7	7.46	1.36	1.31
26	BA	2425	A	C8-N7	7.46	1.36	1.31
26	BA	2560	A	C8-N7	7.46	1.36	1.31
1	AA	459	A	C8-N7	7.45	1.36	1.31
26	BA	10	A	C8-N7	7.45	1.36	1.31
26	BA	1175	A	C8-N7	7.45	1.36	1.31
26	BA	1745	A	C8-N7	7.45	1.36	1.31
26	BA	1791	A	C8-N7	7.45	1.36	1.31
26	BA	2749	A	C8-N7	7.45	1.36	1.31
26	BA	2358	A	C8-N7	7.45	1.36	1.31
26	BA	1614	A	C8-N7	7.45	1.36	1.31
26	BA	1762	A	C8-N7	7.45	1.36	1.31
26	BA	2095	A	C8-N7	7.45	1.36	1.31
26	BA	2776	A	C8-N7	7.45	1.36	1.31
1	AA	329	A	C8-N7	7.45	1.36	1.31
1	AA	371	A	C8-N7	7.45	1.36	1.31
26	BA	415	A	C8-N7	7.45	1.36	1.31
26	BA	2052	A	C8-N7	7.45	1.36	1.31
26	BA	877	A	C8-N7	7.45	1.36	1.31
1	AA	872	A	C8-N7	7.45	1.36	1.31
1	AA	1398	A	C8-N7	7.45	1.36	1.31
22	AV	19	A	C8-N7	7.45	1.36	1.31
26	BA	21	A	C8-N7	7.45	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	920	A	C8-N7	7.45	1.36	1.31
1	AA	923	A	C8-N7	7.44	1.36	1.31
1	AA	1350	A	C8-N7	7.44	1.36	1.31
26	BA	706	A	C8-N7	7.44	1.36	1.31
26	BA	2887	A	C8-N7	7.44	1.36	1.31
1	AA	510	A	C8-N7	7.44	1.36	1.31
26	BA	1783	A	C8-N7	7.44	1.36	1.31
1	AA	873	A	C8-N7	7.44	1.36	1.31
26	BA	28	A	C8-N7	7.44	1.36	1.31
26	BA	1829	A	C8-N7	7.44	1.36	1.31
26	BA	2635	A	C8-N7	7.44	1.36	1.31
26	BA	2706	A	C8-N7	7.44	1.36	1.31
1	AA	1022	A	C8-N7	7.44	1.36	1.31
26	BA	146	A	C8-N7	7.44	1.36	1.31
26	BA	1328	A	C8-N7	7.44	1.36	1.31
26	BA	1635	A	C8-N7	7.44	1.36	1.31
26	BA	2311	A	C8-N7	7.44	1.36	1.31
26	BA	2426	A	C8-N7	7.44	1.36	1.31
1	AA	900	A	C8-N7	7.43	1.36	1.31
26	BA	2080	A	C8-N7	7.43	1.36	1.31
26	BA	2171	A	C8-N7	7.43	1.36	1.31
1	AA	205	A	C8-N7	7.43	1.36	1.31
26	BA	959	A	C8-N7	7.43	1.36	1.31
26	BA	1801	A	C8-N7	7.43	1.36	1.31
26	BA	2058	A	C8-N7	7.43	1.36	1.31
26	BA	2366	A	C8-N7	7.43	1.36	1.31
1	AA	729	A	C8-N7	7.43	1.36	1.31
1	AA	270	A	C8-N7	7.43	1.36	1.31
1	AA	621	A	C8-N7	7.43	1.36	1.31
1	AA	1035	A	C8-N7	7.43	1.36	1.31
26	BA	95	A	C8-N7	7.43	1.36	1.31
26	BA	127	A	C8-N7	7.43	1.36	1.31
26	BA	502	A	C8-N7	7.43	1.36	1.31
26	BA	1598	A	C8-N7	7.43	1.36	1.31
26	BA	2014	A	C8-N7	7.43	1.36	1.31
25	AY	66	A	C8-N7	7.43	1.36	1.31
26	BA	1583	A	C8-N7	7.43	1.36	1.31
26	BA	1700	A	C8-N7	7.43	1.36	1.31
26	BA	1953	A	C8-N7	7.43	1.36	1.31
1	AA	109	A	C8-N7	7.43	1.36	1.31
26	BA	1387	A	C8-N7	7.43	1.36	1.31
26	BA	2547	A	C8-N7	7.43	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2765	A	C8-N7	7.43	1.36	1.31
26	BA	2778	A	C8-N7	7.43	1.36	1.31
26	BA	2856	A	C8-N7	7.43	1.36	1.31
26	BA	49	A	C8-N7	7.42	1.36	1.31
26	BA	56	A	C8-N7	7.42	1.36	1.31
26	BA	429	A	C8-N7	7.42	1.36	1.31
26	BA	675	A	C8-N7	7.42	1.36	1.31
1	AA	1044	A	C8-N7	7.42	1.36	1.31
1	AA	1318	A	C8-N7	7.42	1.36	1.31
26	BA	981	A	C8-N7	7.42	1.36	1.31
26	BA	1393	A	C8-N7	7.42	1.36	1.31
26	BA	586	A	C8-N7	7.42	1.36	1.31
1	AA	1252	A	C8-N7	7.42	1.36	1.31
1	AA	1299	A	C8-N7	7.42	1.36	1.31
26	BA	1535	A	C8-N7	7.42	1.36	1.31
26	BA	430	A	C8-N7	7.42	1.36	1.31
1	AA	1483	A	C8-N7	7.42	1.36	1.31
1	AA	968	A	C8-N7	7.41	1.36	1.31
26	BA	1395	A	C8-N7	7.41	1.36	1.31
26	BA	2826	A	C8-N7	7.41	1.36	1.31
26	BA	1260	A	C8-N7	7.41	1.36	1.31
26	BA	2675	A	C8-N7	7.41	1.36	1.31
26	BA	255	A	C8-N7	7.41	1.36	1.31
26	BA	2407	A	C8-N7	7.41	1.36	1.31
1	AA	1429	A	C8-N7	7.41	1.36	1.31
26	BA	401	A	C8-N7	7.41	1.36	1.31
26	BA	793	A	C8-N7	7.41	1.36	1.31
26	BA	1549	A	C8-N7	7.41	1.36	1.31
26	BA	794	A	C8-N7	7.40	1.36	1.31
26	BA	197	A	C8-N7	7.40	1.36	1.31
26	BA	984	A	C8-N7	7.40	1.36	1.31
26	BA	756	A	C8-N7	7.40	1.36	1.31
1	AA	640	A	C8-N7	7.40	1.36	1.31
26	BA	1365	A	C8-N7	7.40	1.36	1.31
27	BB	45	A	C8-N7	7.40	1.36	1.31
26	BA	1439	A	C8-N7	7.39	1.36	1.31
26	BA	1276	A	C8-N7	7.39	1.36	1.31
26	BA	685	A	C8-N7	7.39	1.36	1.31
1	AA	908	A	C8-N7	7.39	1.36	1.31
26	BA	2386	A	C8-N7	7.39	1.36	1.31
26	BA	1241	A	C8-N7	7.39	1.36	1.31
26	BA	1787	A	C8-N7	7.39	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1219	A	C8-N7	7.38	1.36	1.31
26	BA	63	A	C8-N7	7.38	1.36	1.31
1	AA	162	A	C8-N7	7.38	1.36	1.31
23	AW	23	A	C8-N7	7.38	1.36	1.31
26	BA	447	A	C8-N7	7.38	1.36	1.31
26	BA	705	A	C8-N7	7.38	1.36	1.31
26	BA	2051	A	C8-N7	7.38	1.36	1.31
26	BA	2823	A	C8-N7	7.38	1.36	1.31
26	BA	470	A	C8-N7	7.38	1.36	1.31
26	BA	1809	A	C8-N7	7.38	1.36	1.31
25	AY	23	A	C8-N7	7.38	1.36	1.31
26	BA	1244	A	C8-N7	7.38	1.36	1.31
26	BA	743	A	C8-N7	7.38	1.36	1.31
1	AA	509	A	C8-N7	7.37	1.36	1.31
23	AW	20	U	C2-N3	7.37	1.43	1.37
26	BA	2335	A	C8-N7	7.37	1.36	1.31
1	AA	1339	A	C8-N7	7.37	1.36	1.31
26	BA	820	A	C8-N7	7.37	1.36	1.31
26	BA	1969	A	C8-N7	7.37	1.36	1.31
1	AA	907	A	C8-N7	7.37	1.36	1.31
26	BA	513	A	C8-N7	7.37	1.36	1.31
26	BA	863	A	C8-N7	7.37	1.36	1.31
26	BA	1664	A	C8-N7	7.37	1.36	1.31
26	BA	2082	A	C8-N7	7.37	1.36	1.31
26	BA	2531	A	C8-N7	7.37	1.36	1.31
1	AA	1357	A	C8-N7	7.36	1.36	1.31
26	BA	190	A	C8-N7	7.36	1.36	1.31
26	BA	2800	A	C8-N7	7.36	1.36	1.31
26	BA	2328	A	C8-N7	7.36	1.36	1.31
26	BA	384	A	C8-N7	7.36	1.36	1.31
26	BA	1669	A	C8-N7	7.36	1.36	1.31
26	BA	1810	A	C8-N7	7.35	1.36	1.31
1	AA	546	A	C8-N7	7.35	1.36	1.31
26	BA	466	A	C8-N7	7.35	1.36	1.31
26	BA	572	A	C8-N7	7.35	1.36	1.31
1	AA	1363	A	C8-N7	7.35	1.36	1.31
26	BA	196	A	C8-N7	7.35	1.36	1.31
26	BA	532	A	C8-N7	7.35	1.36	1.31
26	BA	2459	A	C8-N7	7.34	1.36	1.31
1	AA	1157	A	C8-N7	7.34	1.36	1.31
1	AA	983	A	C8-N7	7.34	1.36	1.31
26	BA	2598	A	C8-N7	7.34	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	994	A	C8-N7	7.33	1.36	1.31
1	AA	814	A	C8-N7	7.33	1.36	1.31
26	BA	1784	A	C8-N7	7.33	1.36	1.31
26	BA	471	A	C8-N7	7.33	1.36	1.31
1	AA	1152	A	C8-N7	7.32	1.36	1.31
26	BA	1553	A	C8-N7	7.32	1.36	1.31
26	BA	1301	A	C8-N7	7.31	1.36	1.31
1	AA	1468	A	C8-N7	7.31	1.36	1.31
26	BA	52	A	C8-N7	7.31	1.36	1.31
26	BA	142	A	C8-N7	7.31	1.36	1.31
1	AA	563	A	C8-N7	7.31	1.36	1.31
1	AA	865	A	C8-N7	7.30	1.36	1.31
26	BA	2287	A	C8-N7	7.30	1.36	1.31
26	BA	1866	A	C8-N7	7.30	1.36	1.31
26	BA	2748	A	C8-N7	7.29	1.36	1.31
1	AA	1167	A	C8-N7	7.29	1.36	1.31
27	BB	59	A	C8-N7	7.29	1.36	1.31
26	BA	251	A	C8-N7	7.28	1.36	1.31
26	BA	1899	A	C8-N7	7.28	1.36	1.31
26	BA	2267	A	C8-N7	7.28	1.36	1.31
26	BA	2077	A	C8-N7	7.28	1.36	1.31
1	AA	300	A	C8-N7	7.28	1.36	1.31
1	AA	608	A	C8-N7	7.28	1.36	1.31
26	BA	933	A	C8-N7	7.27	1.36	1.31
26	BA	2766	A	C8-N7	7.27	1.36	1.31
24	AX	19	U	C2-N3	7.27	1.42	1.37
26	BA	1029	A	C8-N7	7.27	1.36	1.31
26	BA	1213	A	C8-N7	7.27	1.36	1.31
1	AA	1374	A	C8-N7	7.26	1.36	1.31
24	AX	16	U	C2-N3	7.26	1.42	1.37
26	BA	960	A	C8-N7	7.26	1.36	1.31
1	AA	502	A	C8-N7	7.26	1.36	1.31
26	BA	479	A	C8-N7	7.25	1.36	1.31
1	AA	1418	A	C8-N7	7.25	1.36	1.31
26	BA	644	A	C8-N7	7.24	1.36	1.31
26	BA	819	A	C8-N7	7.24	1.36	1.31
1	AA	190	A	C8-N7	7.24	1.36	1.31
1	AA	397	A	C8-N7	7.24	1.36	1.31
26	BA	330	A	C8-N7	7.23	1.36	1.31
1	AA	1102	A	C8-N7	7.23	1.36	1.31
26	BA	2662	A	C8-N7	7.23	1.36	1.31
26	BA	278	A	C8-N7	7.22	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2114	A	C8-N7	7.21	1.36	1.31
26	BA	1970	A	C8-N7	7.21	1.36	1.31
26	BA	2297	A	C8-N7	7.21	1.36	1.31
1	AA	1005	A	C8-N7	7.18	1.36	1.31
24	AX	20	U	C2-N3	7.17	1.42	1.37
26	BA	2430	A	C8-N7	7.16	1.36	1.31
1	AA	901	A	C8-N7	7.12	1.36	1.31
26	BA	1570	A	C8-N7	7.07	1.36	1.31
1	AA	983	A	N3-C4	7.02	1.39	1.34
26	BA	633	A	C8-N7	7.00	1.36	1.31
26	BA	2114	A	N3-C4	6.97	1.39	1.34
26	BA	278	A	N3-C4	6.92	1.39	1.34
1	AA	408	A	C8-N7	6.88	1.36	1.31
26	BA	532	A	N3-C4	6.81	1.39	1.34
1	AA	1167	A	N3-C4	6.79	1.39	1.34
1	AA	116	A	N3-C4	6.79	1.39	1.34
26	BA	2297	A	N3-C4	6.77	1.39	1.34
26	BA	1490	A	N3-C4	6.76	1.39	1.34
26	BA	1301	A	N3-C4	6.75	1.39	1.34
26	BA	1901	A	N3-C4	6.75	1.39	1.34
26	BA	362	A	N3-C4	6.74	1.38	1.34
26	BA	1669	A	N3-C4	6.73	1.38	1.34
26	BA	2287	A	N3-C4	6.73	1.38	1.34
27	BB	73	A	N3-C4	6.72	1.38	1.34
26	BA	1876	A	N3-C4	6.70	1.38	1.34
26	BA	196	A	N3-C4	6.70	1.38	1.34
26	BA	111	A	N3-C4	6.70	1.38	1.34
26	BA	404	A	N3-C4	6.69	1.38	1.34
26	BA	2766	A	N3-C4	6.69	1.38	1.34
26	BA	756	A	N3-C4	6.68	1.38	1.34
26	BA	1535	A	N3-C4	6.68	1.38	1.34
26	BA	1591	A	N3-C4	6.68	1.38	1.34
1	AA	872	A	N3-C4	6.67	1.38	1.34
26	BA	2706	A	N3-C4	6.67	1.38	1.34
26	BA	279	A	N3-C4	6.67	1.38	1.34
26	BA	1583	A	N3-C4	6.67	1.38	1.34
1	AA	468	A	N3-C4	6.66	1.38	1.34
1	AA	270	A	N3-C4	6.65	1.38	1.34
1	AA	389	A	N3-C4	6.65	1.38	1.34
26	BA	1175	A	N3-C4	6.65	1.38	1.34
26	BA	2077	A	N3-C4	6.65	1.38	1.34
1	AA	1196	A	N3-C4	6.65	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	439	A	N3-C4	6.65	1.38	1.34
26	BA	460	A	N3-C4	6.65	1.38	1.34
26	BA	2267	A	N3-C4	6.65	1.38	1.34
26	BA	2211	A	N3-C4	6.65	1.38	1.34
1	AA	1093	A	N3-C4	6.65	1.38	1.34
27	BB	99	A	N3-C4	6.65	1.38	1.34
1	AA	1105	A	N3-C4	6.64	1.38	1.34
26	BA	933	A	N3-C4	6.64	1.38	1.34
26	BA	1244	A	N3-C4	6.64	1.38	1.34
26	BA	2430	A	N3-C4	6.64	1.38	1.34
1	AA	397	A	N3-C4	6.64	1.38	1.34
26	BA	1608	A	N3-C4	6.64	1.38	1.34
1	AA	665	A	N3-C4	6.64	1.38	1.34
26	BA	131	A	N3-C4	6.64	1.38	1.34
26	BA	866	A	N3-C4	6.64	1.38	1.34
26	BA	1469	A	N3-C4	6.63	1.38	1.34
26	BA	2471	A	N3-C4	6.63	1.38	1.34
1	AA	55	A	N3-C4	6.63	1.38	1.34
26	BA	2657	A	N3-C4	6.63	1.38	1.34
1	AA	478	A	N3-C4	6.63	1.38	1.34
26	BA	1048	A	N3-C4	6.63	1.38	1.34
1	AA	1019	A	N3-C4	6.63	1.38	1.34
26	BA	547	A	N3-C4	6.63	1.38	1.34
1	AA	1465	A	N3-C4	6.62	1.38	1.34
26	BA	1745	A	N3-C4	6.62	1.38	1.34
1	AA	366	A	N3-C4	6.62	1.38	1.34
26	BA	149	A	N3-C4	6.62	1.38	1.34
26	BA	644	A	N3-C4	6.62	1.38	1.34
26	BA	2799	A	N3-C4	6.62	1.38	1.34
1	AA	994	A	N3-C4	6.62	1.38	1.34
1	AA	77	A	N3-C4	6.62	1.38	1.34
1	AA	371	A	N3-C4	6.62	1.38	1.34
26	BA	2813	A	N3-C4	6.62	1.38	1.34
23	AW	58	A	N3-C4	6.62	1.38	1.34
1	AA	746	A	N3-C4	6.61	1.38	1.34
1	AA	1441	A	N3-C4	6.61	1.38	1.34
1	AA	1476	A	N3-C4	6.61	1.38	1.34
1	AA	1493	A	N3-C4	6.61	1.38	1.34
1	AA	65	A	N3-C4	6.61	1.38	1.34
26	BA	1503	A	N3-C4	6.61	1.38	1.34
1	AA	155	A	N3-C4	6.61	1.38	1.34
1	AA	364	A	N3-C4	6.61	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	142	A	N3-C4	6.61	1.38	1.34
26	BA	231	A	N3-C4	6.61	1.38	1.34
1	AA	1004	A	N3-C4	6.61	1.38	1.34
1	AA	162	A	N3-C4	6.60	1.38	1.34
1	AA	228	A	N3-C4	6.60	1.38	1.34
26	BA	1268	A	N3-C4	6.60	1.38	1.34
1	AA	782	A	N3-C4	6.60	1.38	1.34
26	BA	330	A	N3-C4	6.60	1.38	1.34
26	BA	1020	A	N3-C4	6.60	1.38	1.34
26	BA	1937	A	N3-C4	6.60	1.38	1.34
23	AW	59	A	N3-C4	6.60	1.38	1.34
26	BA	1090	A	N3-C4	6.60	1.38	1.34
26	BA	1739	A	N3-C4	6.60	1.38	1.34
26	BA	2823	A	N3-C4	6.60	1.38	1.34
26	BA	722	A	N3-C4	6.60	1.38	1.34
26	BA	1111	A	N3-C4	6.60	1.38	1.34
26	BA	1494	A	N3-C4	6.60	1.38	1.34
26	BA	1919	A	N3-C4	6.60	1.38	1.34
1	AA	98	A	N3-C4	6.59	1.38	1.34
1	AA	196	A	N3-C4	6.59	1.38	1.34
26	BA	449	A	N3-C4	6.59	1.38	1.34
26	BA	716	A	N3-C4	6.59	1.38	1.34
26	BA	2600	A	N3-C4	6.59	1.38	1.34
26	BA	2765	A	N3-C4	6.59	1.38	1.34
1	AA	1368	A	N3-C4	6.59	1.38	1.34
25	AY	58	A	N3-C4	6.59	1.38	1.34
26	BA	1027	A	N3-C4	6.59	1.38	1.34
26	BA	1367	A	N3-C4	6.59	1.38	1.34
26	BA	1889	A	N3-C4	6.59	1.38	1.34
26	BA	2660	A	N3-C4	6.59	1.38	1.34
26	BA	689	A	N3-C4	6.59	1.38	1.34
26	BA	1848	A	N3-C4	6.59	1.38	1.34
1	AA	383	A	N3-C4	6.59	1.38	1.34
1	AA	482	A	N3-C4	6.59	1.38	1.34
26	BA	412	A	N3-C4	6.59	1.38	1.34
26	BA	845	A	N3-C4	6.59	1.38	1.34
26	BA	1626	A	N3-C4	6.59	1.38	1.34
26	BA	2191	A	N3-C4	6.59	1.38	1.34
26	BA	2587	A	N3-C4	6.59	1.38	1.34
1	AA	712	A	N3-C4	6.59	1.38	1.34
1	AA	1346	A	N3-C4	6.59	1.38	1.34
26	BA	6	A	N3-C4	6.59	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1829	A	N3-C4	6.59	1.38	1.34
26	BA	2757	A	N3-C4	6.59	1.38	1.34
1	AA	373	A	N3-C4	6.58	1.38	1.34
1	AA	938	A	N3-C4	6.58	1.38	1.34
26	BA	2406	A	N3-C4	6.58	1.38	1.34
26	BA	340	A	N3-C4	6.58	1.38	1.34
26	BA	715	A	N3-C4	6.58	1.38	1.34
26	BA	1088	A	N3-C4	6.58	1.38	1.34
26	BA	1189	A	N3-C4	6.58	1.38	1.34
26	BA	2899	A	N3-C4	6.58	1.38	1.34
1	AA	532	A	N3-C4	6.58	1.38	1.34
1	AA	1324	A	N3-C4	6.58	1.38	1.34
26	BA	925	A	N3-C4	6.58	1.38	1.34
26	BA	1103	A	N3-C4	6.58	1.38	1.34
26	BA	2478	A	N3-C4	6.58	1.38	1.34
1	AA	1042	A	N3-C4	6.58	1.38	1.34
1	AA	946	A	N3-C4	6.58	1.38	1.34
26	BA	272	A	N3-C4	6.58	1.38	1.34
26	BA	1784	A	N3-C4	6.58	1.38	1.34
26	BA	2184	A	N3-C4	6.58	1.38	1.34
1	AA	1036	A	N3-C4	6.57	1.38	1.34
24	AX	26	A	N3-C4	6.57	1.38	1.34
25	AY	69	A	N3-C4	6.57	1.38	1.34
26	BA	64	A	N3-C4	6.57	1.38	1.34
26	BA	173	A	N3-C4	6.57	1.38	1.34
26	BA	984	A	N3-C4	6.57	1.38	1.34
26	BA	1194	A	N3-C4	6.57	1.38	1.34
26	BA	1858	A	N3-C4	6.57	1.38	1.34
26	BA	2062	A	N3-C4	6.57	1.38	1.34
1	AA	461	A	N3-C4	6.57	1.38	1.34
1	AA	602	A	N3-C4	6.57	1.38	1.34
1	AA	845	A	N3-C4	6.57	1.38	1.34
1	AA	1311	A	N3-C4	6.57	1.38	1.34
26	BA	666	A	N3-C4	6.57	1.38	1.34
1	AA	448	A	N3-C4	6.57	1.38	1.34
1	AA	1299	A	N3-C4	6.57	1.38	1.34
26	BA	909	A	N3-C4	6.57	1.38	1.34
26	BA	1126	A	N3-C4	6.57	1.38	1.34
26	BA	1395	A	N3-C4	6.57	1.38	1.34
26	BA	1853	A	N3-C4	6.57	1.38	1.34
26	BA	1938	A	N3-C4	6.57	1.38	1.34
26	BA	2461	A	N3-C4	6.57	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1287	A	N3-C4	6.57	1.38	1.34
26	BA	282	A	N3-C4	6.57	1.38	1.34
1	AA	7	A	N3-C4	6.57	1.38	1.34
1	AA	441	A	N3-C4	6.57	1.38	1.34
1	AA	451	A	N3-C4	6.57	1.38	1.34
26	BA	1262	A	N3-C4	6.57	1.38	1.34
26	BA	1307	A	N3-C4	6.57	1.38	1.34
26	BA	2176	A	N3-C4	6.57	1.38	1.34
26	BA	2634	A	N3-C4	6.57	1.38	1.34
1	AA	101	A	N3-C4	6.57	1.38	1.34
1	AA	460	A	N3-C4	6.57	1.38	1.34
1	AA	1408	A	N3-C4	6.57	1.38	1.34
1	AA	1430	A	N3-C4	6.57	1.38	1.34
26	BA	1241	A	N3-C4	6.57	1.38	1.34
26	BA	2856	A	N3-C4	6.57	1.38	1.34
1	AA	696	A	N3-C4	6.56	1.38	1.34
26	BA	2560	A	N3-C4	6.56	1.38	1.34
1	AA	465	A	N3-C4	6.56	1.38	1.34
26	BA	504	A	N3-C4	6.56	1.38	1.34
26	BA	2205	A	N3-C4	6.56	1.38	1.34
26	BA	2750	A	N3-C4	6.56	1.38	1.34
27	BB	59	A	N3-C4	6.56	1.38	1.34
27	BB	66	A	N3-C4	6.56	1.38	1.34
1	AA	382	A	N3-C4	6.56	1.38	1.34
22	AV	22	A	N3-C4	6.56	1.38	1.34
23	AW	23	A	N3-C4	6.56	1.38	1.34
26	BA	614	A	N3-C4	6.56	1.38	1.34
1	AA	563	A	N3-C4	6.56	1.38	1.34
26	BA	374	A	N3-C4	6.56	1.38	1.34
26	BA	1365	A	N3-C4	6.56	1.38	1.34
26	BA	1439	A	N3-C4	6.56	1.38	1.34
26	BA	2101	A	N3-C4	6.56	1.38	1.34
26	BA	2376	A	N3-C4	6.56	1.38	1.34
26	BA	1143	A	N3-C4	6.56	1.38	1.34
27	BB	15	A	N3-C4	6.56	1.38	1.34
23	AW	14	A	N3-C4	6.56	1.38	1.34
25	AY	35	A	N3-C4	6.56	1.38	1.34
26	BA	1246	A	N3-C4	6.56	1.38	1.34
1	AA	1046	A	N3-C4	6.55	1.38	1.34
26	BA	706	A	N3-C4	6.55	1.38	1.34
26	BA	2873	A	N3-C4	6.55	1.38	1.34
1	AA	914	A	N3-C4	6.55	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1081	A	N3-C4	6.55	1.38	1.34
1	AA	1157	A	N3-C4	6.55	1.38	1.34
1	AA	1256	A	N3-C4	6.55	1.38	1.34
26	BA	1014	A	N3-C4	6.55	1.38	1.34
1	AA	1180	A	N3-C4	6.55	1.38	1.34
26	BA	21	A	N3-C4	6.55	1.38	1.34
26	BA	401	A	N3-C4	6.55	1.38	1.34
26	BA	415	A	N3-C4	6.55	1.38	1.34
26	BA	602	A	N3-C4	6.55	1.38	1.34
26	BA	1502	A	N3-C4	6.55	1.38	1.34
26	BA	2015	A	N3-C4	6.55	1.38	1.34
26	BA	2288	A	N3-C4	6.55	1.38	1.34
26	BA	2518	A	N3-C4	6.55	1.38	1.34
26	BA	2665	A	N3-C4	6.55	1.38	1.34
1	AA	706	A	N3-C4	6.55	1.38	1.34
1	AA	747	A	N3-C4	6.55	1.38	1.34
1	AA	1012	A	N3-C4	6.55	1.38	1.34
26	BA	844	A	N3-C4	6.55	1.38	1.34
26	BA	1586	A	N3-C4	6.55	1.38	1.34
26	BA	2154	A	N3-C4	6.55	1.38	1.34
26	BA	2868	A	N3-C4	6.55	1.38	1.34
1	AA	596	A	N3-C4	6.55	1.38	1.34
26	BA	2366	A	N3-C4	6.55	1.38	1.34
27	BB	57	A	N3-C4	6.55	1.38	1.34
1	AA	412	A	N3-C4	6.55	1.38	1.34
1	AA	496	A	N3-C4	6.55	1.38	1.34
1	AA	535	A	N3-C4	6.55	1.38	1.34
1	AA	1111	A	N3-C4	6.55	1.38	1.34
26	BA	10	A	N3-C4	6.55	1.38	1.34
26	BA	63	A	N3-C4	6.55	1.38	1.34
26	BA	181	A	N3-C4	6.55	1.38	1.34
26	BA	878	A	N3-C4	6.55	1.38	1.34
26	BA	917	A	N3-C4	6.55	1.38	1.34
26	BA	2095	A	N3-C4	6.55	1.38	1.34
26	BA	2142	A	N3-C4	6.55	1.38	1.34
26	BA	2170	A	N3-C4	6.55	1.38	1.34
26	BA	2247	A	N3-C4	6.55	1.38	1.34
26	BA	2270	A	N3-C4	6.55	1.38	1.34
26	BA	2317	A	N3-C4	6.54	1.38	1.34
1	AA	303	A	N3-C4	6.54	1.38	1.34
1	AA	694	A	N3-C4	6.54	1.38	1.34
1	AA	814	A	N3-C4	6.54	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	152	A	N3-C4	6.54	1.38	1.34
26	BA	384	A	N3-C4	6.54	1.38	1.34
26	BA	2654	A	N3-C4	6.54	1.38	1.34
1	AA	595	A	N3-C4	6.54	1.38	1.34
1	AA	687	A	N3-C4	6.54	1.38	1.34
1	AA	1014	A	N3-C4	6.54	1.38	1.34
26	BA	71	A	N3-C4	6.54	1.38	1.34
26	BA	1096	A	N3-C4	6.54	1.38	1.34
26	BA	1169	A	N3-C4	6.54	1.38	1.34
26	BA	2531	A	N3-C4	6.54	1.38	1.34
1	AA	649	A	N3-C4	6.54	1.38	1.34
26	BA	94	A	N3-C4	6.54	1.38	1.34
26	BA	244	A	N3-C4	6.54	1.38	1.34
26	BA	613	A	N3-C4	6.54	1.38	1.34
26	BA	1050	A	N3-C4	6.54	1.38	1.34
1	AA	704	A	N3-C4	6.54	1.38	1.34
1	AA	1377	A	N3-C4	6.54	1.38	1.34
1	AA	1492	A	N3-C4	6.54	1.38	1.34
26	BA	616	A	N3-C4	6.54	1.38	1.34
26	BA	2459	A	N3-C4	6.54	1.38	1.34
27	BB	115	A	N3-C4	6.54	1.38	1.34
1	AA	1110	A	N3-C4	6.54	1.38	1.34
26	BA	727	A	N3-C4	6.54	1.38	1.34
26	BA	1095	A	N3-C4	6.54	1.38	1.34
26	BA	1247	A	N3-C4	6.54	1.38	1.34
1	AA	728	A	N3-C4	6.54	1.38	1.34
1	AA	1101	A	N3-C4	6.54	1.38	1.34
1	AA	1151	A	N3-C4	6.54	1.38	1.34
26	BA	833	A	N3-C4	6.54	1.38	1.34
26	BA	2060	A	N3-C4	6.54	1.38	1.34
27	BB	53	A	N3-C4	6.54	1.38	1.34
1	AA	3	A	N3-C4	6.53	1.38	1.34
1	AA	59	A	N3-C4	6.53	1.38	1.34
1	AA	246	A	N3-C4	6.53	1.38	1.34
1	AA	306	A	N3-C4	6.53	1.38	1.34
1	AA	743	A	N3-C4	6.53	1.38	1.34
1	AA	794	A	N3-C4	6.53	1.38	1.34
1	AA	977	A	N3-C4	6.53	1.38	1.34
1	AA	1102	A	N3-C4	6.53	1.38	1.34
1	AA	1360	A	N3-C4	6.53	1.38	1.34
23	AW	38	A	N3-C4	6.53	1.38	1.34
24	AX	41	A	N3-C4	6.53	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	693	A	N3-C4	6.53	1.38	1.34
26	BA	1785	A	N3-C4	6.53	1.38	1.34
26	BA	2378	A	N3-C4	6.53	1.38	1.34
26	BA	2800	A	N3-C4	6.53	1.38	1.34
1	AA	487	A	N3-C4	6.53	1.38	1.34
23	AW	26	A	N3-C4	6.53	1.38	1.34
26	BA	1274	A	N3-C4	6.53	1.38	1.34
26	BA	1477	A	N3-C4	6.53	1.38	1.34
26	BA	1637	A	N3-C4	6.53	1.38	1.34
26	BA	2082	A	N3-C4	6.53	1.38	1.34
26	BA	2721	A	N3-C4	6.53	1.38	1.34
1	AA	2	A	N3-C4	6.53	1.38	1.34
1	AA	152	A	N3-C4	6.53	1.38	1.34
1	AA	539	A	N3-C4	6.53	1.38	1.34
1	AA	767	A	N3-C4	6.53	1.38	1.34
1	AA	1021	A	N3-C4	6.53	1.38	1.34
1	AA	1055	A	N3-C4	6.53	1.38	1.34
1	AA	1188	A	N3-C4	6.53	1.38	1.34
24	AX	23	A	N3-C4	6.53	1.38	1.34
26	BA	56	A	N3-C4	6.53	1.38	1.34
26	BA	197	A	N3-C4	6.53	1.38	1.34
26	BA	299	A	N3-C4	6.53	1.38	1.34
26	BA	730	A	N3-C4	6.53	1.38	1.34
26	BA	1070	A	N3-C4	6.53	1.38	1.34
26	BA	1308	A	N3-C4	6.53	1.38	1.34
26	BA	2725	A	N3-C4	6.53	1.38	1.34
27	BB	104	A	N3-C4	6.53	1.38	1.34
1	AA	974	A	N3-C4	6.53	1.38	1.34
26	BA	911	A	N3-C4	6.53	1.38	1.34
26	BA	996	A	N3-C4	6.53	1.38	1.34
26	BA	1265	A	N3-C4	6.53	1.38	1.34
26	BA	1635	A	N3-C4	6.53	1.38	1.34
26	BA	2738	A	N3-C4	6.53	1.38	1.34
27	BB	46	A	N3-C4	6.53	1.38	1.34
1	AA	466	A	N3-C4	6.53	1.38	1.34
25	AY	23	A	N3-C4	6.53	1.38	1.34
26	BA	1640	A	N3-C4	6.53	1.38	1.34
26	BA	1960	A	N3-C4	6.53	1.38	1.34
26	BA	2284	A	N3-C4	6.53	1.38	1.34
26	BA	2352	A	N3-C4	6.53	1.38	1.34
26	BA	2670	A	N3-C4	6.53	1.38	1.34
1	AA	923	A	N3-C4	6.53	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1219	A	N3-C4	6.53	1.38	1.34
1	AA	1288	A	N3-C4	6.53	1.38	1.34
25	AY	21	A	N3-C4	6.53	1.38	1.34
26	BA	144	A	N3-C4	6.53	1.38	1.34
26	BA	447	A	N3-C4	6.53	1.38	1.34
26	BA	472	A	N3-C4	6.53	1.38	1.34
26	BA	1885	A	N3-C4	6.53	1.38	1.34
26	BA	1927	A	N3-C4	6.53	1.38	1.34
26	BA	2534	A	N3-C4	6.53	1.38	1.34
1	AA	1016	A	N3-C4	6.52	1.38	1.34
26	BA	223	A	N3-C4	6.52	1.38	1.34
26	BA	753	A	N3-C4	6.52	1.38	1.34
1	AA	160	A	N3-C4	6.52	1.38	1.34
1	AA	195	A	N3-C4	6.52	1.38	1.34
1	AA	430	A	N3-C4	6.52	1.38	1.34
1	AA	1000	A	N3-C4	6.52	1.38	1.34
1	AA	1349	A	N3-C4	6.52	1.38	1.34
22	AV	17	A	N3-C4	6.52	1.38	1.34
26	BA	207	A	N3-C4	6.52	1.38	1.34
26	BA	1413	A	N3-C4	6.52	1.38	1.34
1	AA	1534	A	N3-C4	6.52	1.38	1.34
1	AA	190	A	N3-C4	6.52	1.38	1.34
1	AA	673	A	N3-C4	6.52	1.38	1.34
1	AA	1434	A	N3-C4	6.52	1.38	1.34
26	BA	354	A	N3-C4	6.52	1.38	1.34
26	BA	900	A	N3-C4	6.52	1.38	1.34
26	BA	1226	A	N3-C4	6.52	1.38	1.34
26	BA	1254	A	N3-C4	6.52	1.38	1.34
26	BA	1570	A	N3-C4	6.52	1.38	1.34
26	BA	2003	A	N3-C4	6.52	1.38	1.34
26	BA	2377	A	N3-C4	6.52	1.38	1.34
1	AA	509	A	N3-C4	6.52	1.38	1.34
1	AA	608	A	N3-C4	6.52	1.38	1.34
1	AA	621	A	N3-C4	6.52	1.38	1.34
1	AA	1508	A	N3-C4	6.52	1.38	1.34
26	BA	575	A	N3-C4	6.52	1.38	1.34
26	BA	626	A	N3-C4	6.52	1.38	1.34
26	BA	1304	A	N3-C4	6.52	1.38	1.34
26	BA	2407	A	N3-C4	6.52	1.38	1.34
26	BA	2764	A	N3-C4	6.52	1.38	1.34
26	BA	2835	A	N3-C4	6.52	1.38	1.34
26	BA	2893	A	N3-C4	6.52	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	431	A	N3-C4	6.52	1.38	1.34
26	BA	721	A	N3-C4	6.52	1.38	1.34
26	BA	1089	A	N3-C4	6.52	1.38	1.34
26	BA	1260	A	N3-C4	6.52	1.38	1.34
26	BA	2173	A	N3-C4	6.52	1.38	1.34
1	AA	1022	A	N3-C4	6.51	1.38	1.34
1	AA	1271	A	N3-C4	6.51	1.38	1.34
26	BA	428	A	N3-C4	6.51	1.38	1.34
26	BA	945	A	N3-C4	6.51	1.38	1.34
26	BA	1230	A	N3-C4	6.51	1.38	1.34
26	BA	1664	A	N3-C4	6.51	1.38	1.34
26	BA	2749	A	N3-C4	6.51	1.38	1.34
1	AA	607	A	N3-C4	6.51	1.38	1.34
1	AA	1503	A	N3-C4	6.51	1.38	1.34
26	BA	483	A	N3-C4	6.51	1.38	1.34
26	BA	739	A	N3-C4	6.51	1.38	1.34
26	BA	1872	A	N3-C4	6.51	1.38	1.34
26	BA	2094	A	N3-C4	6.51	1.38	1.34
1	AA	26	A	N3-C4	6.51	1.38	1.34
1	AA	908	A	N3-C4	6.51	1.38	1.34
1	AA	1229	A	N3-C4	6.51	1.38	1.34
24	AX	3	A	N3-C4	6.51	1.38	1.34
26	BA	529	A	N3-C4	6.51	1.38	1.34
26	BA	1387	A	N3-C4	6.51	1.38	1.34
26	BA	1713	A	N3-C4	6.51	1.38	1.34
26	BA	2826	A	N3-C4	6.51	1.38	1.34
1	AA	149	A	N3-C4	6.51	1.38	1.34
1	AA	784	A	N3-C4	6.51	1.38	1.34
23	AW	31	A	N3-C4	6.51	1.38	1.34
25	AY	9	A	N3-C4	6.51	1.38	1.34
26	BA	443	A	N3-C4	6.51	1.38	1.34
26	BA	1342	A	N3-C4	6.51	1.38	1.34
26	BA	2134	A	N3-C4	6.51	1.38	1.34
1	AA	363	A	N3-C4	6.51	1.38	1.34
1	AA	1146	A	N3-C4	6.51	1.38	1.34
1	AA	1176	A	N3-C4	6.51	1.38	1.34
1	AA	1261	A	N3-C4	6.51	1.38	1.34
26	BA	1553	A	N3-C4	6.51	1.38	1.34
1	AA	161	A	N3-C4	6.51	1.38	1.34
1	AA	648	A	N3-C4	6.51	1.38	1.34
1	AA	907	A	N3-C4	6.51	1.38	1.34
1	AA	1191	A	N3-C4	6.51	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1289	A	N3-C4	6.51	1.38	1.34
1	AA	1350	A	N3-C4	6.51	1.38	1.34
1	AA	1357	A	N3-C4	6.51	1.38	1.34
22	AV	19	A	N3-C4	6.51	1.38	1.34
26	BA	478	A	N3-C4	6.51	1.38	1.34
26	BA	670	A	N3-C4	6.51	1.38	1.34
26	BA	1580	A	N3-C4	6.51	1.38	1.34
26	BA	1616	A	N3-C4	6.51	1.38	1.34
26	BA	1877	A	N3-C4	6.51	1.38	1.34
26	BA	1978	A	N3-C4	6.51	1.38	1.34
26	BA	2198	A	N3-C4	6.51	1.38	1.34
26	BA	2412	A	N3-C4	6.51	1.38	1.34
1	AA	579	A	N3-C4	6.50	1.38	1.34
1	AA	1225	A	N3-C4	6.50	1.38	1.34
26	BA	256	A	N3-C4	6.50	1.38	1.34
26	BA	1603	A	N3-C4	6.50	1.38	1.34
1	AA	71	A	N3-C4	6.50	1.38	1.34
1	AA	130	A	N3-C4	6.50	1.38	1.34
1	AA	236	A	N3-C4	6.50	1.38	1.34
1	AA	309	A	N3-C4	6.50	1.38	1.34
1	AA	715	A	N3-C4	6.50	1.38	1.34
1	AA	937	A	N3-C4	6.50	1.38	1.34
1	AA	1197	A	N3-C4	6.50	1.38	1.34
1	AA	1513	A	N3-C4	6.50	1.38	1.34
25	AY	66	A	N3-C4	6.50	1.38	1.34
26	BA	89	A	N3-C4	6.50	1.38	1.34
26	BA	677	A	N3-C4	6.50	1.38	1.34
26	BA	896	A	N3-C4	6.50	1.38	1.34
26	BA	1098	A	N3-C4	6.50	1.38	1.34
26	BA	1552	A	N3-C4	6.50	1.38	1.34
26	BA	2426	A	N3-C4	6.50	1.38	1.34
26	BA	2887	A	N3-C4	6.50	1.38	1.34
1	AA	262	A	N3-C4	6.50	1.38	1.34
1	AA	338	A	N3-C4	6.50	1.38	1.34
1	AA	676	A	N3-C4	6.50	1.38	1.34
1	AA	815	A	N3-C4	6.50	1.38	1.34
1	AA	1035	A	N3-C4	6.50	1.38	1.34
26	BA	155	A	N3-C4	6.50	1.38	1.34
26	BA	160	A	N3-C4	6.50	1.38	1.34
26	BA	172	A	N3-C4	6.50	1.38	1.34
26	BA	608	A	N3-C4	6.50	1.38	1.34
26	BA	764	A	N3-C4	6.50	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1504	A	N3-C4	6.50	1.38	1.34
26	BA	1505	A	N3-C4	6.50	1.38	1.34
26	BA	2108	A	N3-C4	6.50	1.38	1.34
26	BA	2314	A	N3-C4	6.50	1.38	1.34
26	BA	2369	A	N3-C4	6.50	1.38	1.34
26	BA	2411	A	N3-C4	6.50	1.38	1.34
1	AA	959	A	N3-C4	6.50	1.38	1.34
26	BA	423	A	N3-C4	6.50	1.38	1.34
26	BA	572	A	N3-C4	6.50	1.38	1.34
26	BA	819	A	N3-C4	6.50	1.38	1.34
26	BA	861	A	N3-C4	6.50	1.38	1.34
26	BA	1393	A	N3-C4	6.50	1.38	1.34
26	BA	1698	A	N3-C4	6.50	1.38	1.34
1	AA	559	A	N3-C4	6.50	1.38	1.34
1	AA	1005	A	N3-C4	6.50	1.38	1.34
1	AA	1044	A	N3-C4	6.50	1.38	1.34
1	AA	1318	A	N3-C4	6.50	1.38	1.34
1	AA	1433	A	N3-C4	6.50	1.38	1.34
23	AW	51	A	N3-C4	6.50	1.38	1.34
26	BA	538	A	N3-C4	6.50	1.38	1.34
26	BA	820	A	N3-C4	6.50	1.38	1.34
26	BA	1866	A	N3-C4	6.50	1.38	1.34
1	AA	553	A	N3-C4	6.50	1.38	1.34
1	AA	878	A	N3-C4	6.50	1.38	1.34
1	AA	909	A	N3-C4	6.50	1.38	1.34
1	AA	1306	A	N3-C4	6.50	1.38	1.34
26	BA	631	A	N3-C4	6.50	1.38	1.34
26	BA	1054	A	N3-C4	6.50	1.38	1.34
26	BA	1508	A	N3-C4	6.50	1.38	1.34
26	BA	1590	A	N3-C4	6.50	1.38	1.34
26	BA	1918	A	N3-C4	6.50	1.38	1.34
26	BA	2097	A	N3-C4	6.50	1.38	1.34
27	BB	109	A	N3-C4	6.50	1.38	1.34
1	AA	139	A	N3-C4	6.50	1.38	1.34
1	AA	1340	A	N3-C4	6.50	1.38	1.34
1	AA	1431	A	N3-C4	6.50	1.38	1.34
26	BA	347	A	N3-C4	6.50	1.38	1.34
26	BA	502	A	N3-C4	6.50	1.38	1.34
1	AA	72	A	N3-C4	6.49	1.38	1.34
1	AA	1257	A	N3-C4	6.49	1.38	1.34
1	AA	1428	A	N3-C4	6.49	1.38	1.34
23	AW	69	A	N3-C4	6.49	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	146	A	N3-C4	6.49	1.38	1.34
26	BA	528	A	N3-C4	6.49	1.38	1.34
26	BA	632	A	N3-C4	6.49	1.38	1.34
26	BA	751	A	N3-C4	6.49	1.38	1.34
26	BA	1322	A	N3-C4	6.49	1.38	1.34
26	BA	2860	A	N3-C4	6.49	1.38	1.34
27	BB	101	A	N3-C4	6.49	1.38	1.34
24	AX	58	A	N3-C4	6.49	1.38	1.34
26	BA	13	A	N3-C4	6.49	1.38	1.34
26	BA	324	A	N3-C4	6.49	1.38	1.34
26	BA	1080	A	N3-C4	6.49	1.38	1.34
26	BA	1549	A	N3-C4	6.49	1.38	1.34
26	BA	1744	A	N3-C4	6.49	1.38	1.34
26	BA	2346	A	N3-C4	6.49	1.38	1.34
26	BA	2837	A	N3-C4	6.49	1.38	1.34
1	AA	250	A	N3-C4	6.49	1.38	1.34
1	AA	411	A	N3-C4	6.49	1.38	1.34
1	AA	560	A	N3-C4	6.49	1.38	1.34
26	BA	165	A	N3-C4	6.49	1.38	1.34
26	BA	471	A	N3-C4	6.49	1.38	1.34
26	BA	508	A	N3-C4	6.49	1.38	1.34
26	BA	522	A	N3-C4	6.49	1.38	1.34
26	BA	789	A	N3-C4	6.49	1.38	1.34
26	BA	2135	A	N3-C4	6.49	1.38	1.34
26	BA	2879	A	N3-C4	6.49	1.38	1.34
27	BB	94	A	N3-C4	6.49	1.38	1.34
1	AA	253	A	N3-C4	6.49	1.38	1.34
1	AA	787	A	N3-C4	6.49	1.38	1.34
26	BA	19	A	N3-C4	6.49	1.38	1.34
26	BA	556	A	N3-C4	6.49	1.38	1.34
26	BA	892	A	N3-C4	6.49	1.38	1.34
26	BA	1809	A	N3-C4	6.49	1.38	1.34
1	AA	81	A	N3-C4	6.49	1.38	1.34
1	AA	495	A	N3-C4	6.49	1.38	1.34
1	AA	523	A	N3-C4	6.49	1.38	1.34
1	AA	1429	A	N3-C4	6.49	1.38	1.34
1	AA	1447	A	N3-C4	6.49	1.38	1.34
26	BA	95	A	N3-C4	6.49	1.38	1.34
26	BA	470	A	N3-C4	6.49	1.38	1.34
26	BA	1672	A	N3-C4	6.49	1.38	1.34
26	BA	2381	A	N3-C4	6.49	1.38	1.34
26	BA	2635	A	N3-C4	6.49	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	21	A	N3-C4	6.49	1.38	1.34
26	BA	241	A	N3-C4	6.49	1.38	1.34
1	AA	716	A	N3-C4	6.48	1.38	1.34
26	BA	391	A	N3-C4	6.48	1.38	1.34
26	BA	941	A	N3-C4	6.48	1.38	1.34
26	BA	1759	A	N3-C4	6.48	1.38	1.34
1	AA	181	A	N3-C4	6.48	1.38	1.34
1	AA	807	A	N3-C4	6.48	1.38	1.34
1	AA	918	A	N3-C4	6.48	1.38	1.34
26	BA	1525	A	N3-C4	6.48	1.38	1.34
26	BA	1987	A	N3-C4	6.48	1.38	1.34
26	BA	2497	A	N3-C4	6.48	1.38	1.34
27	BB	78	A	N3-C4	6.48	1.38	1.34
1	AA	167	A	N3-C4	6.48	1.38	1.34
26	BA	1328	A	N3-C4	6.48	1.38	1.34
26	BA	2171	A	N3-C4	6.48	1.38	1.34
26	BA	2432	A	N3-C4	6.48	1.38	1.34
26	BA	2530	A	N3-C4	6.48	1.38	1.34
27	BB	29	A	N3-C4	6.48	1.38	1.34
1	AA	1169	A	N3-C4	6.48	1.38	1.34
26	BA	342	A	N3-C4	6.48	1.38	1.34
26	BA	1509	A	N3-C4	6.48	1.38	1.34
26	BA	1787	A	N3-C4	6.48	1.38	1.34
26	BA	2117	A	N3-C4	6.48	1.38	1.34
1	AA	873	A	N3-C4	6.48	1.38	1.34
26	BA	705	A	N3-C4	6.48	1.38	1.34
26	BA	1572	A	N3-C4	6.48	1.38	1.34
26	BA	1711	A	N3-C4	6.48	1.38	1.34
1	AA	889	A	N3-C4	6.48	1.38	1.34
1	AA	1179	A	N3-C4	6.48	1.38	1.34
26	BA	1133	A	N3-C4	6.48	1.38	1.34
26	BA	1571	A	N3-C4	6.48	1.38	1.34
26	BA	1912	A	N3-C4	6.48	1.38	1.34
26	BA	2037	A	N3-C4	6.48	1.38	1.34
26	BA	2482	A	N3-C4	6.48	1.38	1.34
1	AA	900	A	N3-C4	6.47	1.38	1.34
1	AA	1446	A	N3-C4	6.47	1.38	1.34
1	AA	1483	A	N3-C4	6.47	1.38	1.34
24	AX	21	A	N3-C4	6.47	1.38	1.34
26	BA	936	A	N3-C4	6.47	1.38	1.34
26	BA	1434	A	N3-C4	6.47	1.38	1.34
26	BA	1618	A	N3-C4	6.47	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2266	A	N3-C4	6.47	1.38	1.34
26	BA	2418	A	N3-C4	6.47	1.38	1.34
1	AA	53	A	N3-C4	6.47	1.38	1.34
1	AA	1171	A	N3-C4	6.47	1.38	1.34
1	AA	1363	A	N3-C4	6.47	1.38	1.34
26	BA	49	A	N3-C4	6.47	1.38	1.34
26	BA	1276	A	N3-C4	6.47	1.38	1.34
1	AA	274	A	N3-C4	6.47	1.38	1.34
1	AA	753	A	N3-C4	6.47	1.38	1.34
24	AX	76	A	N3-C4	6.47	1.38	1.34
26	BA	1783	A	N3-C4	6.47	1.38	1.34
26	BA	2126	A	N3-C4	6.47	1.38	1.34
1	AA	129	A	N3-C4	6.47	1.38	1.34
1	AA	288	A	N3-C4	6.47	1.38	1.34
1	AA	642	A	N3-C4	6.47	1.38	1.34
1	AA	1468	A	N3-C4	6.47	1.38	1.34
26	BA	216	A	N3-C4	6.47	1.38	1.34
26	BA	1021	A	N3-C4	6.47	1.38	1.34
26	BA	1127	A	N3-C4	6.47	1.38	1.34
26	BA	1156	A	N3-C4	6.47	1.38	1.34
26	BA	1327	A	N3-C4	6.47	1.38	1.34
26	BA	2821	A	N3-C4	6.47	1.38	1.34
26	BA	2900	A	N3-C4	6.47	1.38	1.34
1	AA	182	A	N3-C4	6.47	1.38	1.34
1	AA	520	A	N3-C4	6.47	1.38	1.34
1	AA	1362	A	N3-C4	6.47	1.38	1.34
26	BA	233	A	N3-C4	6.47	1.38	1.34
26	BA	661	A	N3-C4	6.47	1.38	1.34
26	BA	1801	A	N3-C4	6.47	1.38	1.34
26	BA	2711	A	N3-C4	6.47	1.38	1.34
1	AA	456	A	N3-C4	6.47	1.38	1.34
1	AA	681	A	N3-C4	6.47	1.38	1.34
1	AA	1246	A	N3-C4	6.47	1.38	1.34
26	BA	5	A	N3-C4	6.47	1.38	1.34
26	BA	1084	A	N3-C4	6.47	1.38	1.34
26	BA	1641	A	N3-C4	6.47	1.38	1.34
26	BA	1655	A	N3-C4	6.47	1.38	1.34
26	BA	1786	A	N3-C4	6.47	1.38	1.34
26	BA	2225	A	N3-C4	6.47	1.38	1.34
26	BA	2433	A	N3-C4	6.47	1.38	1.34
26	BA	2758	A	N3-C4	6.47	1.38	1.34
1	AA	66	A	N3-C4	6.46	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	80	A	N3-C4	6.46	1.38	1.34
1	AA	729	A	N3-C4	6.46	1.38	1.34
1	AA	1456	A	N3-C4	6.46	1.38	1.34
26	BA	101	A	N3-C4	6.46	1.38	1.34
26	BA	222	A	N3-C4	6.46	1.38	1.34
26	BA	402	A	N3-C4	6.46	1.38	1.34
26	BA	477	A	N3-C4	6.46	1.38	1.34
26	BA	750	A	N3-C4	6.46	1.38	1.34
26	BA	2058	A	N3-C4	6.46	1.38	1.34
26	BA	2453	A	N3-C4	6.46	1.38	1.34
26	BA	2820	A	N3-C4	6.46	1.38	1.34
1	AA	906	A	N3-C4	6.46	1.38	1.34
24	AX	14	A	N3-C4	6.46	1.38	1.34
26	BA	453	A	N3-C4	6.46	1.38	1.34
26	BA	482	A	N3-C4	6.46	1.38	1.34
27	BB	108	A	N3-C4	6.46	1.38	1.34
1	AA	864	A	N3-C4	6.46	1.38	1.34
25	AY	26	A	N3-C4	6.46	1.38	1.34
26	BA	119	A	N3-C4	6.46	1.38	1.34
26	BA	735	A	N3-C4	6.46	1.38	1.34
26	BA	792	A	N3-C4	6.46	1.38	1.34
26	BA	1272	A	N3-C4	6.46	1.38	1.34
26	BA	1899	A	N3-C4	6.46	1.38	1.34
26	BA	2298	A	N3-C4	6.46	1.38	1.34
26	BA	2850	A	N3-C4	6.46	1.38	1.34
1	AA	432	A	N3-C4	6.46	1.38	1.34
1	AA	702	A	N3-C4	6.46	1.38	1.34
24	AX	9	A	N3-C4	6.46	1.38	1.34
26	BA	156	A	N3-C4	6.46	1.38	1.34
26	BA	294	A	N3-C4	6.46	1.38	1.34
26	BA	310	A	N3-C4	6.46	1.38	1.34
26	BA	1735	A	N3-C4	6.46	1.38	1.34
26	BA	2392	A	N3-C4	6.46	1.38	1.34
26	BA	2781	A	N3-C4	6.46	1.38	1.34
1	AA	8	A	N3-C4	6.46	1.38	1.34
1	AA	28	A	N3-C4	6.46	1.38	1.34
1	AA	825	A	N3-C4	6.46	1.38	1.34
1	AA	1201	A	N3-C4	6.46	1.38	1.34
1	AA	1248	A	N3-C4	6.46	1.38	1.34
26	BA	960	A	N3-C4	6.46	1.38	1.34
26	BA	1287	A	N3-C4	6.46	1.38	1.34
26	BA	1366	A	N3-C4	6.46	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1847	A	N3-C4	6.46	1.38	1.34
26	BA	2019	A	N3-C4	6.46	1.38	1.34
1	AA	635	A	N3-C4	6.46	1.38	1.34
1	AA	1280	A	N3-C4	6.46	1.38	1.34
1	AA	1531	A	N3-C4	6.46	1.38	1.34
23	AW	42	A	N3-C4	6.46	1.38	1.34
26	BA	28	A	N3-C4	6.46	1.38	1.34
26	BA	103	A	N3-C4	6.46	1.38	1.34
26	BA	125	A	N3-C4	6.46	1.38	1.34
26	BA	1528	A	N3-C4	6.46	1.38	1.34
26	BA	1808	A	N3-C4	6.46	1.38	1.34
26	BA	1969	A	N3-C4	6.46	1.38	1.34
26	BA	2183	A	N3-C4	6.46	1.38	1.34
26	BA	2675	A	N3-C4	6.46	1.38	1.34
26	BA	2851	A	N3-C4	6.46	1.38	1.34
1	AA	975	A	N3-C4	6.46	1.38	1.34
23	AW	41	A	N3-C4	6.46	1.38	1.34
26	BA	265	A	N3-C4	6.46	1.38	1.34
26	BA	541	A	N3-C4	6.46	1.38	1.34
26	BA	582	A	N3-C4	6.46	1.38	1.34
26	BA	734	A	N3-C4	6.46	1.38	1.34
26	BA	1545	A	N3-C4	6.46	1.38	1.34
26	BA	1597	A	N3-C4	6.46	1.38	1.34
1	AA	356	A	N3-C4	6.45	1.38	1.34
1	AA	781	A	N3-C4	6.45	1.38	1.34
1	AA	865	A	N3-C4	6.45	1.38	1.34
26	BA	213	A	N3-C4	6.45	1.38	1.34
26	BA	492	A	N3-C4	6.45	1.38	1.34
26	BA	621	A	N3-C4	6.45	1.38	1.34
26	BA	821	A	N3-C4	6.45	1.38	1.34
26	BA	877	A	N3-C4	6.45	1.38	1.34
26	BA	990	A	N3-C4	6.45	1.38	1.34
26	BA	1321	A	N3-C4	6.45	1.38	1.34
26	BA	1871	A	N3-C4	6.45	1.38	1.34
26	BA	2013	A	N3-C4	6.45	1.38	1.34
1	AA	315	A	N3-C4	6.45	1.38	1.34
26	BA	430	A	N3-C4	6.45	1.38	1.34
26	BA	1040	A	N3-C4	6.45	1.38	1.34
26	BA	1144	A	N3-C4	6.45	1.38	1.34
26	BA	1427	A	N3-C4	6.45	1.38	1.34
26	BA	2705	A	N3-C4	6.45	1.38	1.34
1	AA	143	A	N3-C4	6.45	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	499	A	N3-C4	6.45	1.38	1.34
1	AA	949	A	N3-C4	6.45	1.38	1.34
1	AA	1250	A	N3-C4	6.45	1.38	1.34
26	BA	332	A	N3-C4	6.45	1.38	1.34
26	BA	432	A	N3-C4	6.45	1.38	1.34
26	BA	643	A	N3-C4	6.45	1.38	1.34
26	BA	1237	A	N3-C4	6.45	1.38	1.34
26	BA	2080	A	N3-C4	6.45	1.38	1.34
26	BA	2199	A	N3-C4	6.45	1.38	1.34
1	AA	32	A	N3-C4	6.45	1.38	1.34
1	AA	640	A	N3-C4	6.45	1.38	1.34
1	AA	1254	A	N3-C4	6.45	1.38	1.34
1	AA	1507	A	N3-C4	6.45	1.38	1.34
1	AA	1519	A	N3-C4	6.45	1.38	1.34
26	BA	311	A	N3-C4	6.45	1.38	1.34
26	BA	742	A	N3-C4	6.45	1.38	1.34
26	BA	1067	A	N3-C4	6.45	1.38	1.34
26	BA	344	A	N3-C4	6.45	1.38	1.34
26	BA	899	A	N3-C4	6.45	1.38	1.34
26	BA	1347	A	N3-C4	6.45	1.38	1.34
26	BA	1679	A	N3-C4	6.45	1.38	1.34
1	AA	78	A	N3-C4	6.45	1.38	1.34
1	AA	583	A	N3-C4	6.45	1.38	1.34
1	AA	802	A	N3-C4	6.45	1.38	1.34
1	AA	1502	A	N3-C4	6.45	1.38	1.34
26	BA	718	A	N3-C4	6.45	1.38	1.34
26	BA	973	A	N3-C4	6.45	1.38	1.34
26	BA	1000	A	N3-C4	6.45	1.38	1.34
26	BA	1433	A	N3-C4	6.45	1.38	1.34
26	BA	2054	A	N3-C4	6.45	1.38	1.34
26	BA	345	A	N3-C4	6.44	1.38	1.34
26	BA	1134	A	N3-C4	6.44	1.38	1.34
26	BA	1204	A	N3-C4	6.44	1.38	1.34
26	BA	2336	A	N3-C4	6.44	1.38	1.34
26	BA	2741	A	N3-C4	6.44	1.38	1.34
1	AA	1152	A	N3-C4	6.44	1.38	1.34
1	AA	1274	A	N3-C4	6.44	1.38	1.34
23	AW	76	A	N3-C4	6.44	1.38	1.34
26	BA	515	A	N3-C4	6.44	1.38	1.34
26	BA	972	A	N3-C4	6.44	1.38	1.34
26	BA	1722	A	N3-C4	6.44	1.38	1.34
1	AA	573	A	N3-C4	6.44	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	663	A	N3-C4	6.44	1.38	1.34
1	AA	915	A	N3-C4	6.44	1.38	1.34
1	AA	969	A	N3-C4	6.44	1.38	1.34
26	BA	348	A	N3-C4	6.44	1.38	1.34
26	BA	505	A	N3-C4	6.44	1.38	1.34
26	BA	1073	A	N3-C4	6.44	1.38	1.34
26	BA	1420	A	N3-C4	6.44	1.38	1.34
26	BA	1754	A	N3-C4	6.44	1.38	1.34
26	BA	2278	A	N3-C4	6.44	1.38	1.34
26	BA	2439	A	N3-C4	6.44	1.38	1.34
27	BB	52	A	N3-C4	6.44	1.38	1.34
1	AA	1067	A	N3-C4	6.44	1.38	1.34
1	AA	1285	A	N3-C4	6.44	1.38	1.34
25	AY	38	A	N3-C4	6.44	1.38	1.34
26	BA	195	A	N3-C4	6.44	1.38	1.34
26	BA	501	A	N3-C4	6.44	1.38	1.34
26	BA	981	A	N3-C4	6.44	1.38	1.34
26	BA	1689	A	N3-C4	6.44	1.38	1.34
26	BA	2147	A	N3-C4	6.44	1.38	1.34
1	AA	174	A	N3-C4	6.44	1.38	1.34
1	AA	199	A	N3-C4	6.44	1.38	1.34
1	AA	282	A	N3-C4	6.44	1.38	1.34
1	AA	344	A	N3-C4	6.44	1.38	1.34
1	AA	790	A	N3-C4	6.44	1.38	1.34
1	AA	1130	A	N3-C4	6.44	1.38	1.34
1	AA	1500	A	N3-C4	6.44	1.38	1.34
25	AY	6	A	N3-C4	6.44	1.38	1.34
26	BA	1077	A	N3-C4	6.44	1.38	1.34
26	BA	1431	A	N3-C4	6.44	1.38	1.34
26	BA	2163	A	N3-C4	6.44	1.38	1.34
26	BA	2761	A	N3-C4	6.44	1.38	1.34
1	AA	393	A	N3-C4	6.44	1.38	1.34
1	AA	533	A	N3-C4	6.44	1.38	1.34
1	AA	600	A	N3-C4	6.44	1.38	1.34
1	AA	819	A	N3-C4	6.44	1.38	1.34
22	AV	15	A	N3-C4	6.44	1.38	1.34
26	BA	270	A	N3-C4	6.44	1.38	1.34
26	BA	590	A	N3-C4	6.44	1.38	1.34
26	BA	2476	A	N3-C4	6.44	1.38	1.34
26	BA	2503	A	N3-C4	6.44	1.38	1.34
26	BA	2590	A	N3-C4	6.44	1.38	1.34
26	BA	2733	A	N3-C4	6.44	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BB	119	A	N3-C4	6.44	1.38	1.34
1	AA	172	A	N3-C4	6.43	1.38	1.34
1	AA	325	A	N3-C4	6.43	1.38	1.34
1	AA	1227	A	N3-C4	6.43	1.38	1.34
1	AA	1396	A	N3-C4	6.43	1.38	1.34
1	AA	1410	A	N3-C4	6.43	1.38	1.34
26	BA	226	A	N3-C4	6.43	1.38	1.34
26	BA	346	A	N3-C4	6.43	1.38	1.34
26	BA	1566	A	N3-C4	6.43	1.38	1.34
26	BA	1690	A	N3-C4	6.43	1.38	1.34
26	BA	1746	A	N3-C4	6.43	1.38	1.34
26	BA	2513	A	N3-C4	6.43	1.38	1.34
26	BA	2734	A	N3-C4	6.43	1.38	1.34
26	BA	371	A	N3-C4	6.43	1.38	1.34
26	BA	503	A	N3-C4	6.43	1.38	1.34
26	BA	1392	A	N3-C4	6.43	1.38	1.34
26	BA	1569	A	N3-C4	6.43	1.38	1.34
26	BA	1803	A	N3-C4	6.43	1.38	1.34
26	BA	2227	A	N3-C4	6.43	1.38	1.34
26	BA	2328	A	N3-C4	6.43	1.38	1.34
26	BA	2727	A	N3-C4	6.43	1.38	1.34
26	BA	2748	A	N3-C4	6.43	1.38	1.34
1	AA	1518	A	N3-C4	6.43	1.38	1.34
26	BA	699	A	N3-C4	6.43	1.38	1.34
1	AA	197	A	N3-C4	6.43	1.38	1.34
1	AA	320	A	N3-C4	6.43	1.38	1.34
1	AA	329	A	N3-C4	6.43	1.38	1.34
1	AA	1204	A	N3-C4	6.43	1.38	1.34
1	AA	1375	A	N3-C4	6.43	1.38	1.34
26	BA	127	A	N3-C4	6.43	1.38	1.34
26	BA	928	A	N3-C4	6.43	1.38	1.34
26	BA	959	A	N3-C4	6.43	1.38	1.34
26	BA	2031	A	N3-C4	6.43	1.38	1.34
26	BA	2088	A	N3-C4	6.43	1.38	1.34
1	AA	298	A	N3-C4	6.43	1.38	1.34
26	BA	352	A	N3-C4	6.43	1.38	1.34
26	BA	654	A	N3-C4	6.43	1.38	1.34
26	BA	2358	A	N3-C4	6.43	1.38	1.34
1	AA	50	A	N3-C4	6.43	1.38	1.34
1	AA	353	A	N3-C4	6.43	1.38	1.34
1	AA	435	A	N3-C4	6.43	1.38	1.34
1	AA	675	A	N3-C4	6.43	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	792	A	N3-C4	6.43	1.38	1.34
1	AA	1480	A	N3-C4	6.43	1.38	1.34
26	BA	14	A	N3-C4	6.43	1.38	1.34
26	BA	255	A	N3-C4	6.43	1.38	1.34
26	BA	943	A	N3-C4	6.43	1.38	1.34
26	BA	988	A	N3-C4	6.43	1.38	1.34
26	BA	1952	A	N3-C4	6.43	1.38	1.34
26	BA	2070	A	N3-C4	6.43	1.38	1.34
26	BA	2268	A	N3-C4	6.43	1.38	1.34
26	BA	2778	A	N3-C4	6.43	1.38	1.34
1	AA	179	A	N3-C4	6.42	1.38	1.34
1	AA	192	A	N3-C4	6.42	1.38	1.34
1	AA	498	A	N3-C4	6.42	1.38	1.34
1	AA	1117	A	N3-C4	6.42	1.38	1.34
1	AA	1499	A	N3-C4	6.42	1.38	1.34
26	BA	176	A	N3-C4	6.42	1.38	1.34
26	BA	507	A	N3-C4	6.42	1.38	1.34
26	BA	849	A	N3-C4	6.42	1.38	1.34
26	BA	980	A	N3-C4	6.42	1.38	1.34
26	BA	1815	A	N3-C4	6.42	1.38	1.34
26	BA	1913	A	N3-C4	6.42	1.38	1.34
26	BA	1998	A	N3-C4	6.42	1.38	1.34
1	AA	718	A	N3-C4	6.42	1.38	1.34
1	AA	759	A	N3-C4	6.42	1.38	1.34
26	BA	1596	A	N3-C4	6.42	1.38	1.34
1	AA	629	A	N3-C4	6.42	1.38	1.34
1	AA	768	A	N3-C4	6.42	1.38	1.34
1	AA	831	A	N3-C4	6.42	1.38	1.34
26	BA	191	A	N3-C4	6.42	1.38	1.34
26	BA	749	A	N3-C4	6.42	1.38	1.34
26	BA	1544	A	N3-C4	6.42	1.38	1.34
26	BA	2434	A	N3-C4	6.42	1.38	1.34
26	BA	2614	A	N3-C4	6.42	1.38	1.34
26	BA	2810	A	N3-C4	6.42	1.38	1.34
26	BA	2886	A	N3-C4	6.42	1.38	1.34
26	BA	91	A	N3-C4	6.42	1.38	1.34
26	BA	480	A	N3-C4	6.42	1.38	1.34
26	BA	627	A	N3-C4	6.42	1.38	1.34
1	AA	313	A	N3-C4	6.42	1.38	1.34
1	AA	780	A	N3-C4	6.42	1.38	1.34
26	BA	42	A	N3-C4	6.42	1.38	1.34
26	BA	262	A	N3-C4	6.42	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	761	A	N3-C4	6.42	1.38	1.34
26	BA	1046	A	N3-C4	6.42	1.38	1.34
26	BA	1069	A	N3-C4	6.42	1.38	1.34
26	BA	1678	A	N3-C4	6.42	1.38	1.34
26	BA	1762	A	N3-C4	6.42	1.38	1.34
26	BA	2281	A	N3-C4	6.42	1.38	1.34
26	BA	2602	A	N3-C4	6.42	1.38	1.34
26	BA	2700	A	N3-C4	6.42	1.38	1.34
1	AA	131	A	N3-C4	6.42	1.38	1.34
26	BA	218	A	N3-C4	6.42	1.38	1.34
26	BA	637	A	N3-C4	6.42	1.38	1.34
26	BA	1205	A	N3-C4	6.42	1.38	1.34
26	BA	1932	A	N3-C4	6.42	1.38	1.34
26	BA	2009	A	N3-C4	6.42	1.38	1.34
26	BA	2311	A	N3-C4	6.42	1.38	1.34
1	AA	996	A	N3-C4	6.42	1.38	1.34
23	AW	66	A	N3-C4	6.42	1.38	1.34
26	BA	429	A	N3-C4	6.42	1.38	1.34
26	BA	782	A	N3-C4	6.42	1.38	1.34
26	BA	1652	A	N3-C4	6.42	1.38	1.34
26	BA	1757	A	N3-C4	6.42	1.38	1.34
26	BA	309	A	N3-C4	6.41	1.38	1.34
26	BA	382	A	N3-C4	6.41	1.38	1.34
26	BA	829	A	N3-C4	6.41	1.38	1.34
26	BA	863	A	N3-C4	6.41	1.38	1.34
26	BA	947	A	N3-C4	6.41	1.38	1.34
26	BA	1057	A	N3-C4	6.41	1.38	1.34
26	BA	1213	A	N3-C4	6.41	1.38	1.34
26	BA	1717	A	N3-C4	6.41	1.38	1.34
26	BA	2565	A	N3-C4	6.41	1.38	1.34
27	BB	34	A	N3-C4	6.41	1.38	1.34
1	AA	205	A	N3-C4	6.41	1.38	1.34
1	AA	300	A	N3-C4	6.41	1.38	1.34
1	AA	493	A	N3-C4	6.41	1.38	1.34
1	AA	749	A	N3-C4	6.41	1.38	1.34
25	AY	14	A	N3-C4	6.41	1.38	1.34
26	BA	633	A	N3-C4	6.41	1.38	1.34
26	BA	1495	A	N3-C4	6.41	1.38	1.34
26	BA	1916	A	N3-C4	6.41	1.38	1.34
1	AA	349	A	N3-C4	6.41	1.38	1.34
1	AA	901	A	N3-C4	6.41	1.38	1.34
26	BA	44	A	N3-C4	6.41	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1284	A	N3-C4	6.41	1.38	1.34
26	BA	1609	A	N3-C4	6.41	1.38	1.34
26	BA	1981	A	N3-C4	6.41	1.38	1.34
26	BA	2014	A	N3-C4	6.41	1.38	1.34
26	BA	2564	A	N3-C4	6.41	1.38	1.34
26	BA	2577	A	N3-C4	6.41	1.38	1.34
26	BA	2589	A	N3-C4	6.41	1.38	1.34
26	BA	2726	A	N3-C4	6.41	1.38	1.34
1	AA	171	A	N3-C4	6.41	1.38	1.34
1	AA	630	A	N3-C4	6.41	1.38	1.34
1	AA	777	A	N3-C4	6.41	1.38	1.34
1	AA	1252	A	N3-C4	6.41	1.38	1.34
26	BA	1269	A	N3-C4	6.41	1.38	1.34
26	BA	1403	A	N3-C4	6.41	1.38	1.34
26	BA	1522	A	N3-C4	6.41	1.38	1.34
26	BA	1789	A	N3-C4	6.41	1.38	1.34
26	BA	2386	A	N3-C4	6.41	1.38	1.34
26	BA	1705	A	N3-C4	6.41	1.38	1.34
26	BA	2516	A	N3-C4	6.41	1.38	1.34
1	AA	119	A	N3-C4	6.41	1.38	1.34
1	AA	223	A	N3-C4	6.41	1.38	1.34
1	AA	1145	A	N3-C4	6.41	1.38	1.34
1	AA	1437	A	N3-C4	6.41	1.38	1.34
26	BA	182	A	N3-C4	6.41	1.38	1.34
26	BA	788	A	N3-C4	6.41	1.38	1.34
26	BA	1009	A	N3-C4	6.41	1.38	1.34
26	BA	1151	A	N3-C4	6.41	1.38	1.34
26	BA	1794	A	N3-C4	6.41	1.38	1.34
26	BA	1970	A	N3-C4	6.41	1.38	1.34
26	BA	2468	A	N3-C4	6.41	1.38	1.34
26	BA	2753	A	N3-C4	6.41	1.38	1.34
1	AA	1275	A	N3-C4	6.40	1.38	1.34
26	BA	74	A	N3-C4	6.40	1.38	1.34
26	BA	563	A	N3-C4	6.40	1.38	1.34
26	BA	2450	A	N3-C4	6.40	1.38	1.34
1	AA	622	A	N3-C4	6.40	1.38	1.34
22	AV	21	A	N3-C4	6.40	1.38	1.34
25	AY	73	A	N3-C4	6.40	1.38	1.34
26	BA	685	A	N3-C4	6.40	1.38	1.34
26	BA	1532	A	N3-C4	6.40	1.38	1.34
26	BA	2119	A	N3-C4	6.40	1.38	1.34
26	BA	2679	A	N3-C4	6.40	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2809	A	N3-C4	6.40	1.38	1.34
26	BA	1302	A	N3-C4	6.40	1.38	1.34
26	BA	1453	A	N3-C4	6.40	1.38	1.34
26	BA	2005	A	N3-C4	6.40	1.38	1.34
26	BA	2059	A	N3-C4	6.40	1.38	1.34
1	AA	1251	A	N3-C4	6.40	1.38	1.34
26	BA	190	A	N3-C4	6.40	1.38	1.34
26	BA	783	A	N3-C4	6.40	1.38	1.34
26	BA	1384	A	N3-C4	6.40	1.38	1.34
1	AA	978	A	N3-C4	6.40	1.38	1.34
26	BA	83	A	N3-C4	6.40	1.38	1.34
26	BA	1821	A	N3-C4	6.40	1.38	1.34
26	BA	2333	A	N3-C4	6.40	1.38	1.34
26	BA	2639	A	N3-C4	6.40	1.38	1.34
1	AA	10	A	N3-C4	6.40	1.38	1.34
1	AA	189	A	N3-C4	6.40	1.38	1.34
26	BA	251	A	N3-C4	6.40	1.38	1.34
26	BA	1515	A	N3-C4	6.40	1.38	1.34
26	BA	1900	A	N3-C4	6.40	1.38	1.34
26	BA	2542	A	N3-C4	6.40	1.38	1.34
1	AA	860	A	N3-C4	6.39	1.38	1.34
26	BA	118	A	N3-C4	6.39	1.38	1.34
26	BA	227	A	N3-C4	6.39	1.38	1.34
26	BA	586	A	N3-C4	6.39	1.38	1.34
26	BA	927	A	N3-C4	6.39	1.38	1.34
26	BA	1470	A	N3-C4	6.39	1.38	1.34
26	BA	1551	A	N3-C4	6.39	1.38	1.34
26	BA	1614	A	N3-C4	6.39	1.38	1.34
26	BA	1634	A	N3-C4	6.39	1.38	1.34
26	BA	2736	A	N3-C4	6.39	1.38	1.34
26	BA	2792	A	N3-C4	6.39	1.38	1.34
1	AA	415	A	N3-C4	6.39	1.38	1.34
26	BA	126	A	N3-C4	6.39	1.38	1.34
26	BA	322	A	N3-C4	6.39	1.38	1.34
26	BA	1496	A	N3-C4	6.39	1.38	1.34
26	BA	1810	A	N3-C4	6.39	1.38	1.34
26	BA	2274	A	N3-C4	6.39	1.38	1.34
26	BA	2309	A	N3-C4	6.39	1.38	1.34
26	BA	2340	A	N3-C4	6.39	1.38	1.34
26	BA	167	A	N3-C4	6.39	1.38	1.34
26	BA	752	A	N3-C4	6.39	1.38	1.34
26	BA	422	A	N3-C4	6.39	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1010	A	N3-C4	6.39	1.38	1.34
26	BA	1359	A	N3-C4	6.39	1.38	1.34
26	BA	2090	A	N3-C4	6.39	1.38	1.34
26	BA	2632	A	N3-C4	6.39	1.38	1.34
1	AA	19	A	N3-C4	6.39	1.38	1.34
26	BA	199	A	N3-C4	6.39	1.38	1.34
26	BA	1749	A	N3-C4	6.39	1.38	1.34
26	BA	2882	A	N3-C4	6.39	1.38	1.34
1	AA	572	A	N3-C4	6.39	1.38	1.34
1	AA	1339	A	N3-C4	6.39	1.38	1.34
26	BA	84	A	N3-C4	6.39	1.38	1.34
26	BA	676	A	N3-C4	6.39	1.38	1.34
26	BA	1285	A	N3-C4	6.39	1.38	1.34
26	BA	1701	A	N3-C4	6.39	1.38	1.34
26	BA	1780	A	N3-C4	6.39	1.38	1.34
26	BA	1928	A	N3-C4	6.39	1.38	1.34
26	BA	2052	A	N3-C4	6.39	1.38	1.34
26	BA	2662	A	N3-C4	6.39	1.38	1.34
27	BB	39	A	N3-C4	6.39	1.38	1.34
1	AA	109	A	N3-C4	6.38	1.38	1.34
1	AA	695	A	N3-C4	6.38	1.38	1.34
1	AA	1333	A	N3-C4	6.38	1.38	1.34
26	BA	794	A	N3-C4	6.38	1.38	1.34
26	BA	800	A	N3-C4	6.38	1.38	1.34
26	BA	1264	A	N3-C4	6.38	1.38	1.34
26	BA	1419	A	N3-C4	6.38	1.38	1.34
26	BA	2335	A	N3-C4	6.38	1.38	1.34
1	AA	1080	A	N3-C4	6.38	1.38	1.34
1	AA	1150	A	N3-C4	6.38	1.38	1.34
1	AA	327	A	N3-C4	6.38	1.38	1.34
1	AA	336	A	N3-C4	6.38	1.38	1.34
23	AW	73	A	N3-C4	6.38	1.38	1.34
26	BA	1085	A	N3-C4	6.38	1.38	1.34
26	BA	1165	A	N3-C4	6.38	1.38	1.34
26	BA	1253	A	N3-C4	6.38	1.38	1.34
26	BA	1579	A	N3-C4	6.38	1.38	1.34
26	BA	1677	A	N3-C4	6.38	1.38	1.34
26	BA	1890	A	N3-C4	6.38	1.38	1.34
26	BA	2273	A	N3-C4	6.38	1.38	1.34
26	BA	2388	A	N3-C4	6.38	1.38	1.34
26	BA	1008	A	N3-C4	6.38	1.38	1.34
26	BA	1029	A	N3-C4	6.38	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2776	A	N3-C4	6.38	1.38	1.34
1	AA	892	A	N3-C4	6.38	1.38	1.34
26	BA	203	A	N3-C4	6.38	1.38	1.34
26	BA	1383	A	N3-C4	6.38	1.38	1.34
26	BA	1632	A	N3-C4	6.38	1.38	1.34
26	BA	1665	A	N3-C4	6.38	1.38	1.34
26	BA	2322	A	N3-C4	6.38	1.38	1.34
1	AA	33	A	N3-C4	6.38	1.38	1.34
1	AA	279	A	N3-C4	6.38	1.38	1.34
1	AA	510	A	N3-C4	6.38	1.38	1.34
1	AA	1163	A	N3-C4	6.38	1.38	1.34
26	BA	204	A	N3-C4	6.38	1.38	1.34
26	BA	1353	A	N3-C4	6.38	1.38	1.34
26	BA	1819	A	N3-C4	6.38	1.38	1.34
26	BA	2547	A	N3-C4	6.38	1.38	1.34
1	AA	1236	A	N3-C4	6.38	1.38	1.34
26	BA	804	A	N3-C4	6.38	1.38	1.34
1	AA	374	A	N3-C4	6.37	1.38	1.34
24	AX	24	A	N3-C4	6.37	1.38	1.34
26	BA	513	A	N3-C4	6.37	1.38	1.34
26	BA	1802	A	N3-C4	6.37	1.38	1.34
1	AA	51	A	N3-C4	6.37	1.38	1.34
1	AA	459	A	N3-C4	6.37	1.38	1.34
26	BA	368	A	N3-C4	6.37	1.38	1.34
26	BA	793	A	N3-C4	6.37	1.38	1.34
26	BA	975	A	N3-C4	6.37	1.38	1.34
26	BA	2425	A	N3-C4	6.37	1.38	1.34
1	AA	958	A	N3-C4	6.37	1.38	1.34
1	AA	1418	A	N3-C4	6.37	1.38	1.34
22	AV	20	A	N3-C4	6.37	1.38	1.34
26	BA	1039	A	N3-C4	6.37	1.38	1.34
27	BB	50	A	N3-C4	6.37	1.38	1.34
1	AA	16	A	N3-C4	6.37	1.38	1.34
1	AA	1213	A	N3-C4	6.37	1.38	1.34
1	AA	1319	A	N3-C4	6.37	1.38	1.34
26	BA	221	A	N3-C4	6.37	1.38	1.34
26	BA	918	A	N3-C4	6.37	1.38	1.34
26	BA	1354	A	N3-C4	6.37	1.38	1.34
26	BA	2042	A	N3-C4	6.37	1.38	1.34
26	BA	2435	A	N3-C4	6.37	1.38	1.34
26	BA	73	A	N3-C4	6.37	1.38	1.34
26	BA	1854	A	N3-C4	6.37	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2158	A	N3-C4	6.37	1.38	1.34
1	AA	1082	A	N3-C4	6.36	1.38	1.34
26	BA	2829	A	N3-C4	6.36	1.38	1.34
1	AA	74	A	N3-C4	6.36	1.38	1.34
1	AA	935	A	N3-C4	6.36	1.38	1.34
26	BA	1336	A	N3-C4	6.36	1.38	1.34
26	BA	1654	A	N3-C4	6.36	1.38	1.34
26	BA	1977	A	N3-C4	6.36	1.38	1.34
26	BA	2327	A	N3-C4	6.36	1.38	1.34
26	BA	454	A	N3-C4	6.36	1.38	1.34
26	BA	1028	A	N3-C4	6.36	1.38	1.34
26	BA	1129	A	N3-C4	6.36	1.38	1.34
26	BA	2169	A	N3-C4	6.36	1.38	1.34
26	BA	2448	A	N3-C4	6.36	1.38	1.34
1	AA	120	A	N3-C4	6.36	1.38	1.34
1	AA	554	A	N3-C4	6.36	1.38	1.34
25	AY	41	A	N3-C4	6.36	1.38	1.34
26	BA	300	A	N3-C4	6.36	1.38	1.34
26	BA	910	A	N3-C4	6.36	1.38	1.34
26	BA	1548	A	N3-C4	6.36	1.38	1.34
26	BA	1593	A	N3-C4	6.36	1.38	1.34
1	AA	238	A	N3-C4	6.35	1.38	1.34
1	AA	546	A	N3-C4	6.35	1.38	1.34
26	BA	825	A	N3-C4	6.35	1.38	1.34
26	BA	1773	A	N3-C4	6.35	1.38	1.34
1	AA	913	A	N3-C4	6.35	1.38	1.34
1	AA	1269	A	N3-C4	6.35	1.38	1.34
1	AA	1332	A	N3-C4	6.35	1.38	1.34
26	BA	104	A	N3-C4	6.35	1.38	1.34
26	BA	743	A	N3-C4	6.35	1.38	1.34
26	BA	1032	A	N3-C4	6.35	1.38	1.34
26	BA	2051	A	N3-C4	6.35	1.38	1.34
26	BA	2872	A	N3-C4	6.35	1.38	1.34
1	AA	243	A	N3-C4	6.35	1.38	1.34
26	BA	1001	A	N3-C4	6.35	1.38	1.34
1	AA	151	A	N3-C4	6.35	1.38	1.34
23	AW	9	A	N3-C4	6.35	1.38	1.34
26	BA	161	A	N3-C4	6.35	1.38	1.34
26	BA	1598	A	N3-C4	6.35	1.38	1.34
26	BA	1755	A	N3-C4	6.35	1.38	1.34
26	BA	2030	A	N3-C4	6.35	1.38	1.34
1	AA	964	A	N3-C4	6.35	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1378	A	N3-C4	6.35	1.38	1.34
26	BA	1650	A	N3-C4	6.35	1.38	1.34
1	AA	655	A	N3-C4	6.34	1.38	1.34
1	AA	968	A	N3-C4	6.34	1.38	1.34
1	AA	1238	A	N3-C4	6.34	1.38	1.34
26	BA	1966	A	N3-C4	6.34	1.38	1.34
26	BA	2212	A	N3-C4	6.34	1.38	1.34
26	BA	603	A	N3-C4	6.34	1.38	1.34
26	BA	905	A	N3-C4	6.34	1.38	1.34
1	AA	1239	A	N3-C4	6.34	1.38	1.34
1	AA	1398	A	N3-C4	6.34	1.38	1.34
26	BA	655	A	N3-C4	6.34	1.38	1.34
1	AA	816	A	N3-C4	6.34	1.38	1.34
26	BA	1373	A	N3-C4	6.34	1.38	1.34
1	AA	408	A	N3-C4	6.34	1.38	1.34
26	BA	320	A	N3-C4	6.34	1.38	1.34
26	BA	2469	A	N3-C4	6.34	1.38	1.34
26	BA	2566	A	N3-C4	6.34	1.38	1.34
26	BA	599	A	N3-C4	6.33	1.38	1.34
1	AA	414	A	N3-C4	6.33	1.38	1.34
26	BA	1286	A	N3-C4	6.33	1.38	1.34
26	BA	1700	A	N3-C4	6.33	1.38	1.34
27	BB	45	A	N3-C4	6.33	1.38	1.34
26	BA	52	A	N3-C4	6.33	1.38	1.34
26	BA	2682	A	N3-C4	6.33	1.38	1.34
1	AA	44	A	N3-C4	6.33	1.38	1.34
26	BA	53	A	N3-C4	6.33	1.38	1.34
26	BA	457	A	N3-C4	6.33	1.38	1.34
26	BA	983	A	N3-C4	6.33	1.38	1.34
26	BA	1142	A	N3-C4	6.33	1.38	1.34
26	BA	1214	A	N3-C4	6.33	1.38	1.34
1	AA	547	A	N3-C4	6.33	1.38	1.34
26	BA	920	A	N3-C4	6.33	1.38	1.34
26	BA	2241	A	N3-C4	6.33	1.38	1.34
1	AA	502	A	N3-C4	6.32	1.38	1.34
1	AA	574	A	N3-C4	6.32	1.38	1.34
1	AA	1394	A	N3-C4	6.32	1.38	1.34
26	BA	2572	A	N3-C4	6.32	1.38	1.34
26	BA	668	A	N3-C4	6.32	1.38	1.34
1	AA	1092	A	N3-C4	6.32	1.38	1.34
1	AA	1374	A	N3-C4	6.32	1.38	1.34
26	BA	497	A	N3-C4	6.32	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2541	A	N3-C4	6.32	1.38	1.34
1	AA	1216	A	N3-C4	6.31	1.38	1.34
1	AA	1413	A	N3-C4	6.31	1.38	1.34
26	BA	574	A	N3-C4	6.31	1.38	1.34
26	BA	1791	A	N3-C4	6.31	1.38	1.34
26	BA	979	A	N3-C4	6.31	1.38	1.34
26	BA	609	A	N3-C4	6.31	1.38	1.34
26	BA	781	A	N3-C4	6.31	1.38	1.34
26	BA	2814	A	N3-C4	6.31	1.38	1.34
1	AA	452	A	N3-C4	6.31	1.38	1.34
26	BA	1668	A	N3-C4	6.31	1.38	1.34
26	BA	2071	A	N3-C4	6.31	1.38	1.34
26	BA	1953	A	N3-C4	6.30	1.38	1.34
26	BA	1936	A	N3-C4	6.30	1.38	1.34
26	BA	675	A	N3-C4	6.30	1.38	1.34
1	AA	609	A	N3-C4	6.30	1.38	1.34
26	BA	2740	A	N3-C4	6.30	1.38	1.34
26	BA	526	A	N3-C4	6.30	1.38	1.34
26	BA	1630	A	N3-C4	6.30	1.38	1.34
1	AA	60	A	N3-C4	6.30	1.38	1.34
26	BA	217	A	N3-C4	6.30	1.38	1.34
26	BA	1147	A	N3-C4	6.30	1.38	1.34
26	BA	1772	A	N3-C4	6.30	1.38	1.34
26	BA	1805	A	N3-C4	6.30	1.38	1.34
26	BA	2033	A	N3-C4	6.29	1.38	1.34
26	BA	1275	A	N3-C4	6.29	1.38	1.34
26	BA	2598	A	N3-C4	6.29	1.38	1.34
1	AA	1155	A	N3-C4	6.28	1.38	1.34
26	BA	1155	A	N3-C4	6.28	1.38	1.34
26	BA	802	A	N3-C4	6.28	1.38	1.34
26	BA	2451	A	N3-C4	6.28	1.38	1.34
26	BA	1385	A	N3-C4	6.28	1.38	1.34
26	BA	38	A	N3-C4	6.28	1.38	1.34
26	BA	1676	A	N3-C4	6.28	1.38	1.34
27	BB	58	A	N3-C4	6.27	1.38	1.34
26	BA	219	A	N3-C4	6.27	1.38	1.34
1	AA	766	A	N3-C4	6.27	1.38	1.34
26	BA	1086	A	N3-C4	6.27	1.38	1.34
26	BA	479	A	N3-C4	6.26	1.38	1.34
1	AA	321	A	N3-C4	6.26	1.38	1.34
1	AA	919	A	N3-C4	6.25	1.38	1.34
26	BA	2883	A	N3-C4	6.23	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	514	A	N3-C4	6.23	1.38	1.34
1	AA	263	A	N3-C4	6.22	1.38	1.34
26	BA	2020	A	N3-C4	6.20	1.38	1.34
26	BA	592	A	N3-C4	6.19	1.38	1.34
1	AA	1329	A	N3-C4	6.18	1.38	1.34
26	BA	466	A	N3-C4	6.17	1.38	1.34
1	AA	1170	A	N3-C4	6.17	1.38	1.34
26	BA	1610	A	N3-C4	6.16	1.38	1.34
26	BA	2077	A	C2-N3	5.27	1.38	1.33
1	AA	397	A	C2-N3	5.23	1.38	1.33
26	BA	1494	A	C2-N3	5.22	1.38	1.33
23	AW	26	A	C2-N3	5.21	1.38	1.33
1	AA	539	A	C2-N3	5.20	1.38	1.33
27	BB	59	A	C2-N3	5.20	1.38	1.33
1	AA	98	A	C2-N3	5.20	1.38	1.33
1	AA	1507	A	C2-N3	5.20	1.38	1.33
1	AA	1102	A	C2-N3	5.20	1.38	1.33
26	BA	633	A	C2-N3	5.18	1.38	1.33
1	AA	1363	A	C2-N3	5.18	1.38	1.33
1	AA	478	A	C2-N3	5.18	1.38	1.33
26	BA	819	A	C2-N3	5.18	1.38	1.33
1	AA	1152	A	C2-N3	5.17	1.38	1.33
26	BA	1664	A	C2-N3	5.17	1.38	1.33
26	BA	2191	A	C2-N3	5.17	1.38	1.33
1	AA	1157	A	C2-N3	5.17	1.38	1.33
1	AA	918	A	C2-N3	5.17	1.38	1.33
1	AA	1374	A	C2-N3	5.17	1.38	1.33
26	BA	1548	A	C2-N3	5.17	1.38	1.33
26	BA	2560	A	C2-N3	5.17	1.38	1.33
26	BA	5	A	C2-N3	5.16	1.38	1.33
1	AA	553	A	C2-N3	5.15	1.38	1.33
23	AW	23	A	C2-N3	5.15	1.38	1.33
1	AA	300	A	C2-N3	5.15	1.38	1.33
1	AA	923	A	C2-N3	5.15	1.38	1.33
1	AA	864	A	C2-N3	5.14	1.38	1.33
24	AX	24	A	C2-N3	5.14	1.38	1.33
1	AA	908	A	C2-N3	5.14	1.38	1.33
1	AA	1476	A	C2-N3	5.14	1.38	1.33
26	BA	599	A	C2-N3	5.13	1.38	1.33
26	BA	2459	A	C2-N3	5.13	1.38	1.33
26	BA	2335	A	C2-N3	5.13	1.38	1.33
26	BA	142	A	C2-N3	5.13	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	706	A	C2-N3	5.13	1.38	1.33
26	BA	2800	A	C2-N3	5.13	1.38	1.33
26	BA	1508	A	C2-N3	5.13	1.38	1.33
26	BA	1069	A	C2-N3	5.13	1.38	1.33
26	BA	2433	A	C2-N3	5.13	1.38	1.33
23	AW	41	A	C2-N3	5.12	1.38	1.33
1	AA	55	A	C2-N3	5.12	1.38	1.33
26	BA	750	A	C2-N3	5.12	1.38	1.33
26	BA	794	A	C2-N3	5.12	1.38	1.33
26	BA	1029	A	C2-N3	5.12	1.38	1.33
26	BA	1549	A	C2-N3	5.12	1.38	1.33
26	BA	2378	A	C2-N3	5.12	1.38	1.33
1	AA	432	A	C2-N3	5.12	1.38	1.33
26	BA	231	A	C2-N3	5.12	1.38	1.33
26	BA	793	A	C2-N3	5.12	1.38	1.33
26	BA	2662	A	C2-N3	5.12	1.38	1.33
26	BA	1848	A	C2-N3	5.11	1.38	1.33
26	BA	2727	A	C2-N3	5.11	1.38	1.33
1	AA	1035	A	C2-N3	5.11	1.38	1.33
1	AA	1306	A	C2-N3	5.11	1.38	1.33
24	AX	23	A	C2-N3	5.11	1.38	1.33
26	BA	56	A	C2-N3	5.11	1.38	1.33
26	BA	1260	A	C2-N3	5.11	1.38	1.33
26	BA	1328	A	C2-N3	5.11	1.38	1.33
1	AA	190	A	C2-N3	5.11	1.38	1.33
26	BA	2173	A	C2-N3	5.11	1.38	1.33
1	AA	33	A	C2-N3	5.11	1.38	1.33
1	AA	1180	A	C2-N3	5.11	1.38	1.33
26	BA	1387	A	C2-N3	5.11	1.38	1.33
26	BA	2439	A	C2-N3	5.11	1.38	1.33
1	AA	223	A	C2-N3	5.11	1.38	1.33
1	AA	448	A	C2-N3	5.10	1.38	1.33
26	BA	402	A	C2-N3	5.10	1.38	1.33
26	BA	1453	A	C2-N3	5.10	1.38	1.33
26	BA	2352	A	C2-N3	5.10	1.38	1.33
1	AA	1044	A	C2-N3	5.10	1.38	1.33
1	AA	1350	A	C2-N3	5.10	1.38	1.33
26	BA	64	A	C2-N3	5.10	1.38	1.33
26	BA	582	A	C2-N3	5.10	1.38	1.33
26	BA	2169	A	C2-N3	5.10	1.38	1.33
26	BA	2273	A	C2-N3	5.10	1.38	1.33
26	BA	1213	A	C2-N3	5.10	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2733	A	C2-N3	5.10	1.38	1.33
26	BA	2799	A	C2-N3	5.10	1.38	1.33
1	AA	642	A	C2-N3	5.10	1.38	1.33
26	BA	507	A	C2-N3	5.10	1.38	1.33
26	BA	2267	A	C2-N3	5.10	1.38	1.33
1	AA	1500	A	C2-N3	5.10	1.38	1.33
26	BA	655	A	C2-N3	5.10	1.38	1.33
26	BA	2014	A	C2-N3	5.10	1.38	1.33
1	AA	938	A	C2-N3	5.10	1.38	1.33
26	BA	1899	A	C2-N3	5.10	1.38	1.33
26	BA	2013	A	C2-N3	5.10	1.38	1.33
27	BB	53	A	C2-N3	5.10	1.38	1.33
1	AA	1171	A	C2-N3	5.09	1.38	1.33
26	BA	52	A	C2-N3	5.09	1.38	1.33
26	BA	644	A	C2-N3	5.09	1.38	1.33
26	BA	933	A	C2-N3	5.09	1.38	1.33
26	BA	1353	A	C2-N3	5.09	1.38	1.33
26	BA	1665	A	C2-N3	5.09	1.38	1.33
1	AA	50	A	C2-N3	5.09	1.38	1.33
1	AA	1019	A	C2-N3	5.09	1.38	1.33
1	AA	53	A	C2-N3	5.09	1.38	1.33
1	AA	790	A	C2-N3	5.09	1.38	1.33
1	AA	1418	A	C2-N3	5.09	1.38	1.33
26	BA	753	A	C2-N3	5.09	1.38	1.33
26	BA	863	A	C2-N3	5.09	1.38	1.33
26	BA	2850	A	C2-N3	5.09	1.38	1.33
26	BA	104	A	C2-N3	5.09	1.38	1.33
26	BA	503	A	C2-N3	5.09	1.38	1.33
26	BA	2309	A	C2-N3	5.09	1.38	1.33
26	BA	2837	A	C2-N3	5.09	1.38	1.33
1	AA	563	A	C2-N3	5.09	1.38	1.33
1	AA	718	A	C2-N3	5.09	1.38	1.33
1	AA	746	A	C2-N3	5.09	1.38	1.33
1	AA	819	A	C2-N3	5.09	1.38	1.33
26	BA	590	A	C2-N3	5.09	1.38	1.33
26	BA	556	A	C2-N3	5.08	1.38	1.33
26	BA	2184	A	C2-N3	5.08	1.38	1.33
25	AY	9	A	C2-N3	5.08	1.38	1.33
26	BA	1095	A	C2-N3	5.08	1.38	1.33
26	BA	1496	A	C2-N3	5.08	1.38	1.33
26	BA	2468	A	C2-N3	5.08	1.38	1.33
27	BB	50	A	C2-N3	5.08	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	344	A	C2-N3	5.08	1.38	1.33
1	AA	414	A	C2-N3	5.08	1.38	1.33
1	AA	546	A	C2-N3	5.08	1.38	1.33
1	AA	649	A	C2-N3	5.08	1.38	1.33
1	AA	1022	A	C2-N3	5.08	1.38	1.33
1	AA	1042	A	C2-N3	5.08	1.38	1.33
26	BA	477	A	C2-N3	5.08	1.38	1.33
26	BA	632	A	C2-N3	5.08	1.38	1.33
26	BA	1133	A	C2-N3	5.08	1.38	1.33
26	BA	2284	A	C2-N3	5.08	1.38	1.33
26	BA	2430	A	C2-N3	5.08	1.38	1.33
26	BA	2547	A	C2-N3	5.08	1.38	1.33
1	AA	435	A	C2-N3	5.08	1.38	1.33
26	BA	689	A	C2-N3	5.08	1.38	1.33
26	BA	829	A	C2-N3	5.08	1.38	1.33
1	AA	3	A	C2-N3	5.08	1.38	1.33
26	BA	332	A	C2-N3	5.08	1.38	1.33
26	BA	368	A	C2-N3	5.08	1.38	1.33
26	BA	1354	A	C2-N3	5.08	1.38	1.33
26	BA	1553	A	C2-N3	5.08	1.38	1.33
27	BB	45	A	C2-N3	5.08	1.38	1.33
1	AA	949	A	C2-N3	5.08	1.38	1.33
26	BA	28	A	C2-N3	5.08	1.38	1.33
26	BA	513	A	C2-N3	5.08	1.38	1.33
26	BA	1247	A	C2-N3	5.08	1.38	1.33
26	BA	1434	A	C2-N3	5.08	1.38	1.33
26	BA	1566	A	C2-N3	5.08	1.38	1.33
1	AA	274	A	C2-N3	5.08	1.38	1.33
1	AA	608	A	C2-N3	5.08	1.38	1.33
1	AA	860	A	C2-N3	5.08	1.38	1.33
25	AY	21	A	C2-N3	5.08	1.38	1.33
26	BA	95	A	C2-N3	5.08	1.38	1.33
26	BA	126	A	C2-N3	5.08	1.38	1.33
26	BA	609	A	C2-N3	5.08	1.38	1.33
26	BA	2407	A	C2-N3	5.08	1.38	1.33
1	AA	199	A	C2-N3	5.07	1.38	1.33
1	AA	695	A	C2-N3	5.07	1.38	1.33
1	AA	792	A	C2-N3	5.07	1.38	1.33
1	AA	907	A	C2-N3	5.07	1.38	1.33
1	AA	1396	A	C2-N3	5.07	1.38	1.33
26	BA	820	A	C2-N3	5.07	1.38	1.33
1	AA	1005	A	C2-N3	5.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	572	A	C2-N3	5.07	1.38	1.33
26	BA	1469	A	C2-N3	5.07	1.38	1.33
26	BA	2142	A	C2-N3	5.07	1.38	1.33
26	BA	2725	A	C2-N3	5.07	1.38	1.33
1	AA	482	A	C2-N3	5.07	1.38	1.33
26	BA	2170	A	C2-N3	5.07	1.38	1.33
26	BA	1008	A	C2-N3	5.07	1.38	1.33
26	BA	1302	A	C2-N3	5.07	1.38	1.33
26	BA	1433	A	C2-N3	5.07	1.38	1.33
26	BA	1805	A	C2-N3	5.07	1.38	1.33
26	BA	2587	A	C2-N3	5.07	1.38	1.33
26	BA	478	A	C2-N3	5.07	1.38	1.33
26	BA	1046	A	C2-N3	5.07	1.38	1.33
26	BA	1284	A	C2-N3	5.07	1.38	1.33
26	BA	1525	A	C2-N3	5.07	1.38	1.33
26	BA	1597	A	C2-N3	5.07	1.38	1.33
26	BA	2471	A	C2-N3	5.07	1.38	1.33
26	BA	2530	A	C2-N3	5.07	1.38	1.33
1	AA	502	A	C2-N3	5.07	1.38	1.33
1	AA	892	A	C2-N3	5.07	1.38	1.33
26	BA	309	A	C2-N3	5.07	1.38	1.33
26	BA	449	A	C2-N3	5.07	1.38	1.33
26	BA	925	A	C2-N3	5.07	1.38	1.33
26	BA	972	A	C2-N3	5.07	1.38	1.33
26	BA	2736	A	C2-N3	5.07	1.38	1.33
26	BA	1395	A	C2-N3	5.06	1.38	1.33
1	AA	487	A	C2-N3	5.06	1.38	1.33
1	AA	802	A	C2-N3	5.06	1.38	1.33
26	BA	172	A	C2-N3	5.06	1.38	1.33
26	BA	340	A	C2-N3	5.06	1.38	1.33
26	BA	432	A	C2-N3	5.06	1.38	1.33
26	BA	990	A	C2-N3	5.06	1.38	1.33
26	BA	1535	A	C2-N3	5.06	1.38	1.33
26	BA	1570	A	C2-N3	5.06	1.38	1.33
26	BA	1634	A	C2-N3	5.06	1.38	1.33
26	BA	1637	A	C2-N3	5.06	1.38	1.33
26	BA	1866	A	C2-N3	5.06	1.38	1.33
26	BA	1952	A	C2-N3	5.06	1.38	1.33
1	AA	408	A	C2-N3	5.06	1.38	1.33
26	BA	470	A	C2-N3	5.06	1.38	1.33
26	BA	2183	A	C2-N3	5.06	1.38	1.33
27	BB	39	A	C2-N3	5.06	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1036	A	C2-N3	5.06	1.38	1.33
23	AW	59	A	C2-N3	5.06	1.38	1.33
26	BA	845	A	C2-N3	5.06	1.38	1.33
26	BA	1269	A	C2-N3	5.06	1.38	1.33
26	BA	2734	A	C2-N3	5.06	1.38	1.33
1	AA	155	A	C2-N3	5.06	1.38	1.33
1	AA	174	A	C2-N3	5.06	1.38	1.33
1	AA	1280	A	C2-N3	5.06	1.38	1.33
26	BA	181	A	C2-N3	5.06	1.38	1.33
26	BA	342	A	C2-N3	5.06	1.38	1.33
26	BA	1640	A	C2-N3	5.06	1.38	1.33
26	BA	1676	A	C2-N3	5.06	1.38	1.33
26	BA	2726	A	C2-N3	5.06	1.38	1.33
26	BA	1103	A	C2-N3	5.06	1.38	1.33
26	BA	1616	A	C2-N3	5.06	1.38	1.33
1	AA	1357	A	C2-N3	5.05	1.38	1.33
26	BA	213	A	C2-N3	5.05	1.38	1.33
26	BA	892	A	C2-N3	5.05	1.38	1.33
26	BA	1301	A	C2-N3	5.05	1.38	1.33
26	BA	1632	A	C2-N3	5.05	1.38	1.33
26	BA	2080	A	C2-N3	5.05	1.38	1.33
26	BA	2171	A	C2-N3	5.05	1.38	1.33
26	BA	2706	A	C2-N3	5.05	1.38	1.33
26	BA	165	A	C2-N3	5.05	1.38	1.33
26	BA	1579	A	C2-N3	5.05	1.38	1.33
26	BA	1717	A	C2-N3	5.05	1.38	1.33
1	AA	19	A	C2-N3	5.05	1.38	1.33
1	AA	270	A	C2-N3	5.05	1.38	1.33
1	AA	383	A	C2-N3	5.05	1.38	1.33
1	AA	743	A	C2-N3	5.05	1.38	1.33
1	AA	1080	A	C2-N3	5.05	1.38	1.33
26	BA	666	A	C2-N3	5.05	1.38	1.33
26	BA	2665	A	C2-N3	5.05	1.38	1.33
1	AA	7	A	C2-N3	5.05	1.38	1.33
1	AA	1483	A	C2-N3	5.05	1.38	1.33
1	AA	1508	A	C2-N3	5.05	1.38	1.33
26	BA	453	A	C2-N3	5.05	1.38	1.33
26	BA	471	A	C2-N3	5.05	1.38	1.33
26	BA	716	A	C2-N3	5.05	1.38	1.33
26	BA	920	A	C2-N3	5.05	1.38	1.33
26	BA	1608	A	C2-N3	5.05	1.38	1.33
26	BA	1801	A	C2-N3	5.05	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1998	A	C2-N3	5.05	1.38	1.33
26	BA	2900	A	C2-N3	5.05	1.38	1.33
1	AA	373	A	C2-N3	5.05	1.38	1.33
1	AA	415	A	C2-N3	5.05	1.38	1.33
1	AA	759	A	C2-N3	5.05	1.38	1.33
26	BA	391	A	C2-N3	5.05	1.38	1.33
26	BA	1204	A	C2-N3	5.05	1.38	1.33
26	BA	1205	A	C2-N3	5.05	1.38	1.33
26	BA	1739	A	C2-N3	5.05	1.38	1.33
26	BA	2054	A	C2-N3	5.05	1.38	1.33
26	BA	2700	A	C2-N3	5.05	1.38	1.33
26	BA	2899	A	C2-N3	5.05	1.38	1.33
1	AA	129	A	C2-N3	5.05	1.38	1.33
1	AA	595	A	C2-N3	5.05	1.38	1.33
1	AA	872	A	C2-N3	5.05	1.38	1.33
1	AA	1219	A	C2-N3	5.05	1.38	1.33
22	AV	15	A	C2-N3	5.05	1.38	1.33
26	BA	74	A	C2-N3	5.05	1.38	1.33
26	BA	2062	A	C2-N3	5.05	1.38	1.33
26	BA	2205	A	C2-N3	5.05	1.38	1.33
26	BA	2298	A	C2-N3	5.05	1.38	1.33
26	BA	2721	A	C2-N3	5.05	1.38	1.33
1	AA	607	A	C2-N3	5.04	1.38	1.33
26	BA	1700	A	C2-N3	5.04	1.38	1.33
26	BA	1701	A	C2-N3	5.04	1.38	1.33
26	BA	2572	A	C2-N3	5.04	1.38	1.33
1	AA	119	A	C2-N3	5.04	1.38	1.33
1	AA	635	A	C2-N3	5.04	1.38	1.33
1	AA	1169	A	C2-N3	5.04	1.38	1.33
1	AA	1274	A	C2-N3	5.04	1.38	1.33
25	AY	6	A	C2-N3	5.04	1.38	1.33
26	BA	49	A	C2-N3	5.04	1.38	1.33
26	BA	330	A	C2-N3	5.04	1.38	1.33
26	BA	1077	A	C2-N3	5.04	1.38	1.33
26	BA	1085	A	C2-N3	5.04	1.38	1.33
26	BA	1134	A	C2-N3	5.04	1.38	1.33
26	BA	2297	A	C2-N3	5.04	1.38	1.33
26	BA	2376	A	C2-N3	5.04	1.38	1.33
27	BB	119	A	C2-N3	5.04	1.38	1.33
1	AA	192	A	C2-N3	5.04	1.38	1.33
1	AA	205	A	C2-N3	5.04	1.38	1.33
1	AA	496	A	C2-N3	5.04	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	609	A	C2-N3	5.04	1.38	1.33
1	AA	621	A	C2-N3	5.04	1.38	1.33
1	AA	1236	A	C2-N3	5.04	1.38	1.33
1	AA	1429	A	C2-N3	5.04	1.38	1.33
26	BA	152	A	C2-N3	5.04	1.38	1.33
26	BA	482	A	C2-N3	5.04	1.38	1.33
26	BA	960	A	C2-N3	5.04	1.38	1.33
26	BA	1241	A	C2-N3	5.04	1.38	1.33
26	BA	1977	A	C2-N3	5.04	1.38	1.33
26	BA	2274	A	C2-N3	5.04	1.38	1.33
26	BA	2541	A	C2-N3	5.04	1.38	1.33
26	BA	2654	A	C2-N3	5.04	1.38	1.33
1	AA	152	A	C2-N3	5.04	1.38	1.33
1	AA	1287	A	C2-N3	5.04	1.38	1.33
24	AX	21	A	C2-N3	5.04	1.38	1.33
25	AY	41	A	C2-N3	5.04	1.38	1.33
26	BA	1027	A	C2-N3	5.04	1.38	1.33
26	BA	2657	A	C2-N3	5.04	1.38	1.33
26	BA	2813	A	C2-N3	5.04	1.38	1.33
1	AA	1468	A	C2-N3	5.04	1.38	1.33
26	BA	734	A	C2-N3	5.04	1.38	1.33
26	BA	1151	A	C2-N3	5.04	1.38	1.33
26	BA	1754	A	C2-N3	5.04	1.38	1.33
26	BA	1815	A	C2-N3	5.04	1.38	1.33
26	BA	2088	A	C2-N3	5.04	1.38	1.33
26	BA	2336	A	C2-N3	5.04	1.38	1.33
26	BA	2602	A	C2-N3	5.04	1.38	1.33
26	BA	2675	A	C2-N3	5.04	1.38	1.33
26	BA	685	A	C2-N3	5.04	1.38	1.33
26	BA	1735	A	C2-N3	5.04	1.38	1.33
1	AA	139	A	C2-N3	5.04	1.38	1.33
1	AA	523	A	C2-N3	5.04	1.38	1.33
1	AA	1251	A	C2-N3	5.04	1.38	1.33
26	BA	928	A	C2-N3	5.04	1.38	1.33
26	BA	2311	A	C2-N3	5.04	1.38	1.33
26	BA	2366	A	C2-N3	5.04	1.38	1.33
26	BA	2482	A	C2-N3	5.04	1.38	1.33
26	BA	2765	A	C2-N3	5.04	1.38	1.33
26	BA	2886	A	C2-N3	5.04	1.38	1.33
1	AA	329	A	C2-N3	5.03	1.38	1.33
1	AA	411	A	C2-N3	5.03	1.38	1.33
1	AA	459	A	C2-N3	5.03	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	560	A	C2-N3	5.03	1.38	1.33
1	AA	1201	A	C2-N3	5.03	1.38	1.33
1	AA	1394	A	C2-N3	5.03	1.38	1.33
1	AA	1447	A	C2-N3	5.03	1.38	1.33
26	BA	190	A	C2-N3	5.03	1.38	1.33
26	BA	1090	A	C2-N3	5.03	1.38	1.33
26	BA	1169	A	C2-N3	5.03	1.38	1.33
26	BA	1762	A	C2-N3	5.03	1.38	1.33
26	BA	2082	A	C2-N3	5.03	1.38	1.33
26	BA	2432	A	C2-N3	5.03	1.38	1.33
26	BA	2758	A	C2-N3	5.03	1.38	1.33
26	BA	2872	A	C2-N3	5.03	1.38	1.33
27	BB	52	A	C2-N3	5.03	1.38	1.33
1	AA	371	A	C2-N3	5.03	1.38	1.33
1	AA	901	A	C2-N3	5.03	1.38	1.33
1	AA	1269	A	C2-N3	5.03	1.38	1.33
26	BA	401	A	C2-N3	5.03	1.38	1.33
26	BA	752	A	C2-N3	5.03	1.38	1.33
26	BA	1746	A	C2-N3	5.03	1.38	1.33
26	BA	2748	A	C2-N3	5.03	1.38	1.33
25	AY	14	A	C2-N3	5.03	1.38	1.33
26	BA	522	A	C2-N3	5.03	1.38	1.33
26	BA	979	A	C2-N3	5.03	1.38	1.33
26	BA	1009	A	C2-N3	5.03	1.38	1.33
26	BA	1175	A	C2-N3	5.03	1.38	1.33
26	BA	1276	A	C2-N3	5.03	1.38	1.33
26	BA	1829	A	C2-N3	5.03	1.38	1.33
26	BA	2134	A	C2-N3	5.03	1.38	1.33
26	BA	2425	A	C2-N3	5.03	1.38	1.33
1	AA	162	A	C2-N3	5.03	1.38	1.33
1	AA	579	A	C2-N3	5.03	1.38	1.33
22	AV	20	A	C2-N3	5.03	1.38	1.33
26	BA	1431	A	C2-N3	5.03	1.38	1.33
26	BA	1877	A	C2-N3	5.03	1.38	1.33
26	BA	2070	A	C2-N3	5.03	1.38	1.33
26	BA	2119	A	C2-N3	5.03	1.38	1.33
26	BA	2682	A	C2-N3	5.03	1.38	1.33
1	AA	143	A	C2-N3	5.03	1.38	1.33
1	AA	704	A	C2-N3	5.03	1.38	1.33
1	AA	816	A	C2-N3	5.03	1.38	1.33
1	AA	1285	A	C2-N3	5.03	1.38	1.33
22	AV	21	A	C2-N3	5.03	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	21	A	C2-N3	5.03	1.38	1.33
26	BA	83	A	C2-N3	5.03	1.38	1.33
26	BA	492	A	C2-N3	5.03	1.38	1.33
26	BA	538	A	C2-N3	5.03	1.38	1.33
26	BA	739	A	C2-N3	5.03	1.38	1.33
26	BA	996	A	C2-N3	5.03	1.38	1.33
26	BA	1144	A	C2-N3	5.03	1.38	1.33
26	BA	1678	A	C2-N3	5.03	1.38	1.33
1	AA	364	A	C2-N3	5.03	1.38	1.33
1	AA	520	A	C2-N3	5.03	1.38	1.33
1	AA	1188	A	C2-N3	5.03	1.38	1.33
1	AA	1339	A	C2-N3	5.03	1.38	1.33
26	BA	14	A	C2-N3	5.03	1.38	1.33
26	BA	182	A	C2-N3	5.03	1.38	1.33
26	BA	706	A	C2-N3	5.03	1.38	1.33
26	BA	756	A	C2-N3	5.03	1.38	1.33
26	BA	1089	A	C2-N3	5.03	1.38	1.33
26	BA	1626	A	C2-N3	5.03	1.38	1.33
26	BA	1970	A	C2-N3	5.03	1.38	1.33
26	BA	2042	A	C2-N3	5.03	1.38	1.33
26	BA	2635	A	C2-N3	5.03	1.38	1.33
26	BA	352	A	C2-N3	5.02	1.38	1.33
26	BA	1572	A	C2-N3	5.02	1.38	1.33
26	BA	2163	A	C2-N3	5.02	1.38	1.33
1	AA	116	A	C2-N3	5.02	1.38	1.33
1	AA	279	A	C2-N3	5.02	1.38	1.33
1	AA	298	A	C2-N3	5.02	1.38	1.33
1	AA	460	A	C2-N3	5.02	1.38	1.33
1	AA	600	A	C2-N3	5.02	1.38	1.33
1	AA	815	A	C2-N3	5.02	1.38	1.33
1	AA	1101	A	C2-N3	5.02	1.38	1.33
1	AA	1518	A	C2-N3	5.02	1.38	1.33
26	BA	255	A	C2-N3	5.02	1.38	1.33
26	BA	529	A	C2-N3	5.02	1.38	1.33
26	BA	643	A	C2-N3	5.02	1.38	1.33
26	BA	1722	A	C2-N3	5.02	1.38	1.33
26	BA	131	A	C2-N3	5.02	1.38	1.33
26	BA	173	A	C2-N3	5.02	1.38	1.33
26	BA	219	A	C2-N3	5.02	1.38	1.33
26	BA	447	A	C2-N3	5.02	1.38	1.33
26	BA	861	A	C2-N3	5.02	1.38	1.33
26	BA	1809	A	C2-N3	5.02	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	282	A	C2-N3	5.02	1.38	1.33
1	AA	510	A	C2-N3	5.02	1.38	1.33
1	AA	547	A	C2-N3	5.02	1.38	1.33
1	AA	583	A	C2-N3	5.02	1.38	1.33
1	AA	681	A	C2-N3	5.02	1.38	1.33
1	AA	794	A	C2-N3	5.02	1.38	1.33
1	AA	969	A	C2-N3	5.02	1.38	1.33
1	AA	1246	A	C2-N3	5.02	1.38	1.33
1	AA	1456	A	C2-N3	5.02	1.38	1.33
26	BA	233	A	C2-N3	5.02	1.38	1.33
26	BA	244	A	C2-N3	5.02	1.38	1.33
26	BA	348	A	C2-N3	5.02	1.38	1.33
26	BA	505	A	C2-N3	5.02	1.38	1.33
26	BA	918	A	C2-N3	5.02	1.38	1.33
26	BA	1084	A	C2-N3	5.02	1.38	1.33
26	BA	1885	A	C2-N3	5.02	1.38	1.33
1	AA	1288	A	C2-N3	5.02	1.38	1.33
26	BA	144	A	C2-N3	5.02	1.38	1.33
26	BA	256	A	C2-N3	5.02	1.38	1.33
26	BA	282	A	C2-N3	5.02	1.38	1.33
26	BA	430	A	C2-N3	5.02	1.38	1.33
26	BA	896	A	C2-N3	5.02	1.38	1.33
26	BA	1872	A	C2-N3	5.02	1.38	1.33
26	BA	1938	A	C2-N3	5.02	1.38	1.33
26	BA	2211	A	C2-N3	5.02	1.38	1.33
26	BA	2461	A	C2-N3	5.02	1.38	1.33
1	AA	532	A	C2-N3	5.02	1.38	1.33
1	AA	994	A	C2-N3	5.02	1.38	1.33
1	AA	1519	A	C2-N3	5.02	1.38	1.33
26	BA	730	A	C2-N3	5.02	1.38	1.33
26	BA	917	A	C2-N3	5.02	1.38	1.33
26	BA	2317	A	C2-N3	5.02	1.38	1.33
26	BA	2369	A	C2-N3	5.02	1.38	1.33
26	BA	2792	A	C2-N3	5.02	1.38	1.33
1	AA	59	A	C2-N3	5.01	1.38	1.33
1	AA	325	A	C2-N3	5.01	1.38	1.33
1	AA	456	A	C2-N3	5.01	1.38	1.33
1	AA	1021	A	C2-N3	5.01	1.38	1.33
1	AA	1271	A	C2-N3	5.01	1.38	1.33
1	AA	1318	A	C2-N3	5.01	1.38	1.33
1	AA	1434	A	C2-N3	5.01	1.38	1.33
26	BA	374	A	C2-N3	5.01	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	428	A	C2-N3	5.01	1.38	1.33
26	BA	603	A	C2-N3	5.01	1.38	1.33
26	BA	833	A	C2-N3	5.01	1.38	1.33
26	BA	1528	A	C2-N3	5.01	1.38	1.33
26	BA	1745	A	C2-N3	5.01	1.38	1.33
26	BA	2003	A	C2-N3	5.01	1.38	1.33
26	BA	2095	A	C2-N3	5.01	1.38	1.33
26	BA	2531	A	C2-N3	5.01	1.38	1.33
1	AA	629	A	C2-N3	5.01	1.38	1.33
1	AA	900	A	C2-N3	5.01	1.38	1.33
1	AA	1332	A	C2-N3	5.01	1.38	1.33
1	AA	1410	A	C2-N3	5.01	1.38	1.33
26	BA	160	A	C2-N3	5.01	1.38	1.33
26	BA	637	A	C2-N3	5.01	1.38	1.33
26	BA	1244	A	C2-N3	5.01	1.38	1.33
26	BA	2340	A	C2-N3	5.01	1.38	1.33
26	BA	2518	A	C2-N3	5.01	1.38	1.33
1	AA	161	A	C2-N3	5.01	1.38	1.33
1	AA	189	A	C2-N3	5.01	1.38	1.33
1	AA	320	A	C2-N3	5.01	1.38	1.33
1	AA	533	A	C2-N3	5.01	1.38	1.33
1	AA	640	A	C2-N3	5.01	1.38	1.33
1	AA	1503	A	C2-N3	5.01	1.38	1.33
23	AW	38	A	C2-N3	5.01	1.38	1.33
26	BA	155	A	C2-N3	5.01	1.38	1.33
26	BA	575	A	C2-N3	5.01	1.38	1.33
26	BA	1419	A	C2-N3	5.01	1.38	1.33
26	BA	1618	A	C2-N3	5.01	1.38	1.33
26	BA	1690	A	C2-N3	5.01	1.38	1.33
26	BA	1698	A	C2-N3	5.01	1.38	1.33
26	BA	1847	A	C2-N3	5.01	1.38	1.33
26	BA	2660	A	C2-N3	5.01	1.38	1.33
1	AA	288	A	C2-N3	5.01	1.38	1.33
1	AA	353	A	C2-N3	5.01	1.38	1.33
1	AA	1004	A	C2-N3	5.01	1.38	1.33
1	AA	1117	A	C2-N3	5.01	1.38	1.33
1	AA	1319	A	C2-N3	5.01	1.38	1.33
26	BA	73	A	C2-N3	5.01	1.38	1.33
26	BA	176	A	C2-N3	5.01	1.38	1.33
26	BA	614	A	C2-N3	5.01	1.38	1.33
26	BA	1127	A	C2-N3	5.01	1.38	1.33
26	BA	1495	A	C2-N3	5.01	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	1689	A	C2-N3	5.01	1.38	1.33
26	BA	2386	A	C2-N3	5.01	1.38	1.33
26	BA	2821	A	C2-N3	5.01	1.38	1.33
1	AA	250	A	C2-N3	5.01	1.38	1.33
1	AA	306	A	C2-N3	5.01	1.38	1.33
1	AA	441	A	C2-N3	5.01	1.38	1.33
26	BA	1039	A	C2-N3	5.01	1.38	1.33
26	BA	1889	A	C2-N3	5.01	1.38	1.33
1	AA	262	A	C2-N3	5.01	1.38	1.33
1	AA	466	A	C2-N3	5.01	1.38	1.33
1	AA	1196	A	C2-N3	5.01	1.38	1.33
1	AA	1256	A	C2-N3	5.01	1.38	1.33
1	AA	1311	A	C2-N3	5.01	1.38	1.33
1	AA	1324	A	C2-N3	5.01	1.38	1.33
1	AA	1375	A	C2-N3	5.01	1.38	1.33
1	AA	1430	A	C2-N3	5.01	1.38	1.33
26	BA	6	A	C2-N3	5.01	1.38	1.33
26	BA	19	A	C2-N3	5.01	1.38	1.33
26	BA	167	A	C2-N3	5.01	1.38	1.33
26	BA	661	A	C2-N3	5.01	1.38	1.33
26	BA	693	A	C2-N3	5.01	1.38	1.33
26	BA	2516	A	C2-N3	5.01	1.38	1.33
26	BA	2776	A	C2-N3	5.01	1.38	1.33
26	BA	2826	A	C2-N3	5.01	1.38	1.33
27	BB	101	A	C2-N3	5.01	1.38	1.33
27	BB	115	A	C2-N3	5.01	1.38	1.33
1	AA	172	A	C2-N3	5.00	1.38	1.33
1	AA	535	A	C2-N3	5.00	1.38	1.33
1	AA	675	A	C2-N3	5.00	1.38	1.33
1	AA	1362	A	C2-N3	5.00	1.38	1.33
26	BA	563	A	C2-N3	5.00	1.38	1.33
26	BA	2679	A	C2-N3	5.00	1.38	1.33
1	AA	465	A	C2-N3	5.00	1.38	1.33
1	AA	596	A	C2-N3	5.00	1.38	1.33
1	AA	766	A	C2-N3	5.00	1.38	1.33
1	AA	1012	A	C2-N3	5.00	1.38	1.33
1	AA	1257	A	C2-N3	5.00	1.38	1.33
24	AX	14	A	C2-N3	5.00	1.38	1.33
26	BA	324	A	C2-N3	5.00	1.38	1.33
26	BA	1020	A	C2-N3	5.00	1.38	1.33
26	BA	1304	A	C2-N3	5.00	1.38	1.33
26	BA	2564	A	C2-N3	5.00	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2639	A	C2-N3	5.00	1.38	1.33
1	AA	78	A	C2-N3	5.00	1.38	1.33
1	AA	716	A	C2-N3	5.00	1.38	1.33
1	AA	768	A	C2-N3	5.00	1.38	1.33
1	AA	975	A	C2-N3	5.00	1.38	1.33
1	AA	1093	A	C2-N3	5.00	1.38	1.33
24	AX	3	A	C2-N3	5.00	1.38	1.33
26	BA	103	A	C2-N3	5.00	1.38	1.33
26	BA	196	A	C2-N3	5.00	1.38	1.33
26	BA	439	A	C2-N3	5.00	1.38	1.33
26	BA	460	A	C2-N3	5.00	1.38	1.33
26	BA	504	A	C2-N3	5.00	1.38	1.33
26	BA	1098	A	C2-N3	5.00	1.38	1.33
26	BA	1551	A	C2-N3	5.00	1.38	1.33
26	BA	2051	A	C2-N3	5.00	1.38	1.33
26	BA	2094	A	C2-N3	5.00	1.38	1.33
26	BA	2158	A	C2-N3	5.00	1.38	1.33
26	BA	2281	A	C2-N3	5.00	1.38	1.33
26	BA	2287	A	C2-N3	5.00	1.38	1.33
26	BA	2328	A	C2-N3	5.00	1.38	1.33
26	BA	2534	A	C2-N3	5.00	1.38	1.33
26	BA	2632	A	C2-N3	5.00	1.38	1.33
26	BA	2873	A	C2-N3	5.00	1.38	1.33
26	BA	2893	A	C2-N3	5.00	1.38	1.33
27	BB	66	A	C2-N3	5.00	1.38	1.33

All (14665) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	278	A	C2-N3-C4	20.42	120.81	110.60
1	AA	983	A	C2-N3-C4	20.30	120.75	110.60
26	BA	2114	A	C2-N3-C4	20.19	120.70	110.60
26	BA	514	A	C2-N3-C4	19.99	120.60	110.60
26	BA	2451	A	N1-C6-N6	-19.89	106.67	118.60
26	BA	532	A	C2-N3-C4	19.85	120.53	110.60
26	BA	1378	A	N1-C6-N6	-19.82	106.71	118.60
26	BA	1669	A	C2-N3-C4	19.74	120.47	110.60
1	AA	452	A	N1-C6-N6	-19.62	106.83	118.60
26	BA	1876	A	N1-C6-N6	-19.60	106.84	118.60
1	AA	397	A	C2-N3-C4	19.58	120.39	110.60
26	BA	2765	A	C2-N3-C4	19.57	120.39	110.60
1	AA	622	A	N1-C6-N6	-19.53	106.88	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1301	A	C2-N3-C4	19.50	120.35	110.60
26	BA	2287	A	C2-N3-C4	19.46	120.33	110.60
26	BA	119	A	N1-C6-N6	-19.46	106.92	118.60
1	AA	171	A	N1-C6-N6	-19.44	106.93	118.60
26	BA	1021	A	C2-N3-C4	19.44	120.32	110.60
26	BA	2267	A	C2-N3-C4	19.43	120.32	110.60
1	AA	1167	A	C2-N3-C4	19.43	120.31	110.60
26	BA	2430	A	C2-N3-C4	19.42	120.31	110.60
26	BA	1901	A	C2-N3-C4	19.42	120.31	110.60
26	BA	514	A	N1-C2-N3	-19.42	119.59	129.30
26	BA	514	A	N1-C6-N6	-19.42	106.95	118.60
1	AA	1225	A	N1-C6-N6	-19.41	106.95	118.60
26	BA	1535	A	C2-N3-C4	19.39	120.30	110.60
1	AA	977	A	C2-N3-C4	19.39	120.29	110.60
26	BA	1785	A	N1-C6-N6	-19.36	106.99	118.60
1	AA	1225	A	C2-N3-C4	19.35	120.27	110.60
26	BA	1876	A	C2-N3-C4	19.34	120.27	110.60
1	AA	1299	A	C2-N3-C4	19.34	120.27	110.60
26	BA	2451	A	C2-N3-C4	19.34	120.27	110.60
1	AA	766	A	N1-C6-N6	-19.33	107.00	118.60
26	BA	621	A	N1-C6-N6	-19.32	107.00	118.60
1	AA	872	A	C2-N3-C4	19.31	120.26	110.60
1	AA	563	A	C2-N3-C4	19.31	120.25	110.60
1	AA	1329	A	N1-C6-N6	-19.29	107.02	118.60
1	AA	151	A	N1-C6-N6	-19.28	107.03	118.60
1	AA	889	A	N1-C6-N6	-19.28	107.03	118.60
26	BA	1583	A	C2-N3-C4	19.28	120.24	110.60
26	BA	1214	A	C2-N3-C4	19.26	120.23	110.60
26	BA	2297	A	C2-N3-C4	19.26	120.23	110.60
26	BA	1630	A	N1-C6-N6	-19.26	107.05	118.60
26	BA	404	A	C2-N3-C4	19.25	120.23	110.60
26	BA	1000	A	C2-N3-C4	19.24	120.22	110.60
26	BA	362	A	C2-N3-C4	19.24	120.22	110.60
27	BB	78	A	N1-C6-N6	-19.23	107.06	118.60
26	BA	53	A	N1-C6-N6	-19.23	107.06	118.60
26	BA	2062	A	C2-N3-C4	19.22	120.21	110.60
26	BA	160	A	C2-N3-C4	19.22	120.21	110.60
26	BA	2033	A	N1-C6-N6	-19.21	107.07	118.60
26	BA	371	A	C2-N3-C4	19.21	120.21	110.60
26	BA	2740	A	C2-N3-C4	19.21	120.20	110.60
1	AA	411	A	N1-C6-N6	-19.19	107.08	118.60
26	BA	2589	A	N1-C6-N6	-19.19	107.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1353	A	C2-N3-C4	19.18	120.19	110.60
1	AA	116	A	C2-N3-C4	19.18	120.19	110.60
26	BA	783	A	N1-C6-N6	-19.18	107.09	118.60
26	BA	119	A	N1-C2-N3	-19.18	119.71	129.30
26	BA	910	A	C2-N3-C4	19.18	120.19	110.60
26	BA	2764	A	N1-C6-N6	-19.18	107.09	118.60
26	BA	1919	A	C2-N3-C4	19.18	120.19	110.60
1	AA	389	A	C2-N3-C4	19.18	120.19	110.60
26	BA	802	A	C2-N3-C4	19.18	120.19	110.60
26	BA	1086	A	C2-N3-C4	19.17	120.19	110.60
1	AA	782	A	C2-N3-C4	19.17	120.19	110.60
26	BA	1014	A	N1-C6-N6	-19.17	107.10	118.60
26	BA	1147	A	N1-C6-N6	-19.17	107.10	118.60
26	BA	2766	A	C2-N3-C4	19.17	120.18	110.60
26	BA	1901	A	N1-C6-N6	-19.16	107.10	118.60
1	AA	665	A	N1-C6-N6	-19.15	107.11	118.60
27	BB	59	A	C2-N3-C4	19.14	120.17	110.60
26	BA	2322	A	N1-C6-N6	-19.14	107.12	118.60
27	BB	78	A	C2-N3-C4	19.14	120.17	110.60
1	AA	431	A	N1-C6-N6	-19.14	107.12	118.60
26	BA	1378	A	N1-C2-N3	-19.14	119.73	129.30
26	BA	457	A	N1-C6-N6	-19.13	107.12	118.60
1	AA	622	A	C2-N3-C4	19.13	120.16	110.60
27	BB	34	A	N1-C6-N6	-19.12	107.12	118.60
1	AA	151	A	C2-N3-C4	19.12	120.16	110.60
1	AA	1225	A	N1-C2-N3	-19.12	119.74	129.30
27	BB	73	A	C2-N3-C4	19.12	120.16	110.60
26	BA	1784	A	C2-N3-C4	19.12	120.16	110.60
26	BA	1040	A	N1-C6-N6	-19.11	107.13	118.60
26	BA	1635	A	C2-N3-C4	19.11	120.16	110.60
1	AA	130	A	C2-N3-C4	19.11	120.16	110.60
26	BA	2418	A	N1-C6-N6	-19.11	107.13	118.60
1	AA	435	A	C2-N3-C4	19.10	120.15	110.60
1	AA	1170	A	N1-C6-N6	-19.09	107.14	118.60
1	AA	1333	A	N1-C6-N6	-19.09	107.14	118.60
26	BA	371	A	N1-C6-N6	-19.09	107.14	118.60
26	BA	2469	A	N1-C2-N3	-19.09	119.75	129.30
27	BB	15	A	C2-N3-C4	19.09	120.15	110.60
1	AA	994	A	C2-N3-C4	19.09	120.14	110.60
1	AA	1150	A	N1-C6-N6	-19.09	107.15	118.60
26	BA	196	A	C2-N3-C4	19.09	120.14	110.60
26	BA	905	A	N1-C6-N6	-19.09	107.15	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	468	A	C2-N3-C4	19.09	120.14	110.60
1	AA	554	A	N1-C6-N6	-19.09	107.15	118.60
26	BA	207	A	N1-C6-N6	-19.09	107.15	118.60
26	BA	1088	A	C2-N3-C4	19.09	120.14	110.60
1	AA	782	A	N1-C6-N6	-19.08	107.15	118.60
26	BA	1966	A	C2-N3-C4	19.08	120.14	110.60
1	AA	1332	A	C2-N3-C4	19.08	120.14	110.60
26	BA	1545	A	N1-C6-N6	-19.08	107.15	118.60
26	BA	1378	A	C2-N3-C4	19.07	120.14	110.60
26	BA	1490	A	C2-N3-C4	19.07	120.13	110.60
23	AW	42	A	N1-C6-N6	-19.07	107.16	118.60
1	AA	622	A	N1-C2-N3	-19.06	119.77	129.30
26	BA	547	A	C2-N3-C4	19.06	120.13	110.60
1	AA	195	A	N1-C6-N6	-19.06	107.17	118.60
1	AA	918	A	C2-N3-C4	19.06	120.13	110.60
26	BA	1809	A	C2-N3-C4	19.06	120.13	110.60
1	AA	1333	A	C2-N3-C4	19.05	120.13	110.60
26	BA	217	A	C2-N3-C4	19.05	120.13	110.60
23	AW	26	A	C2-N3-C4	19.05	120.13	110.60
26	BA	384	A	C2-N3-C4	19.05	120.12	110.60
26	BA	2809	A	C2-N3-C4	19.05	120.12	110.60
1	AA	98	A	C2-N3-C4	19.05	120.12	110.60
26	BA	1385	A	N1-C6-N6	-19.05	107.17	118.60
26	BA	654	A	C2-N3-C4	19.05	120.12	110.60
1	AA	1531	A	C2-N3-C4	19.04	120.12	110.60
26	BA	454	A	N1-C6-N6	-19.04	107.17	118.60
26	BA	5	A	C2-N3-C4	19.04	120.12	110.60
26	BA	279	A	C2-N3-C4	19.04	120.12	110.60
26	BA	299	A	C2-N3-C4	19.04	120.12	110.60
1	AA	74	A	N1-C6-N6	-19.03	107.18	118.60
26	BA	204	A	N1-C6-N6	-19.03	107.18	118.60
26	BA	2560	A	C2-N3-C4	19.03	120.12	110.60
1	AA	393	A	N1-C6-N6	-19.03	107.18	118.60
1	AA	579	A	C2-N3-C4	19.03	120.11	110.60
1	AA	1437	A	N1-C2-N3	-19.03	119.79	129.30
26	BA	1876	A	N1-C2-N3	-19.03	119.79	129.30
26	BA	2070	A	C2-N3-C4	19.03	120.11	110.60
26	BA	2450	A	C2-N3-C4	19.03	120.11	110.60
1	AA	546	A	C2-N3-C4	19.02	120.11	110.60
26	BA	1204	A	N1-C6-N6	-19.02	107.19	118.60
26	BA	2451	A	N1-C2-N3	-19.02	119.79	129.30
26	BA	2469	A	N1-C6-N6	-19.02	107.19	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	918	A	C2-N3-C4	19.02	120.11	110.60
26	BA	1262	A	C2-N3-C4	19.02	120.11	110.60
26	BA	2657	A	C2-N3-C4	19.02	120.11	110.60
26	BA	453	A	C2-N3-C4	19.02	120.11	110.60
26	BA	1189	A	C2-N3-C4	19.02	120.11	110.60
26	BA	1365	A	C2-N3-C4	19.01	120.11	110.60
1	AA	499	A	N1-C2-N3	-19.01	119.79	129.30
26	BA	1427	A	N1-C6-N6	-19.01	107.19	118.60
26	BA	371	A	N1-C2-N3	-19.01	119.80	129.30
26	BA	382	A	C2-N3-C4	19.01	120.11	110.60
26	BA	503	A	C2-N3-C4	19.01	120.11	110.60
26	BA	2450	A	N1-C2-N3	-19.01	119.80	129.30
26	BA	1744	A	C2-N3-C4	19.00	120.10	110.60
26	BA	1392	A	C2-N3-C4	19.00	120.10	110.60
26	BA	1230	A	C2-N3-C4	19.00	120.10	110.60
26	BA	1970	A	C2-N3-C4	19.00	120.10	110.60
26	BA	1385	A	N1-C2-N3	-19.00	119.80	129.30
26	BA	2134	A	N1-C6-N6	-19.00	107.20	118.60
1	AA	1227	A	N1-C2-N3	-19.00	119.80	129.30
26	BA	621	A	C2-N3-C4	19.00	120.10	110.60
26	BA	1496	A	C2-N3-C4	19.00	120.10	110.60
26	BA	2518	A	C2-N3-C4	19.00	120.10	110.60
26	BA	119	A	C2-N3-C4	19.00	120.10	110.60
26	BA	592	A	C2-N3-C4	19.00	120.10	110.60
26	BA	2225	A	N1-C6-N6	-19.00	107.20	118.60
1	AA	1151	A	N1-C2-N3	-18.99	119.80	129.30
26	BA	2154	A	N1-C6-N6	-18.99	107.20	118.60
26	BA	56	A	C2-N3-C4	18.99	120.09	110.60
1	AA	487	A	C2-N3-C4	18.99	120.09	110.60
26	BA	480	A	C2-N3-C4	18.99	120.09	110.60
26	BA	909	A	C2-N3-C4	18.99	120.09	110.60
26	BA	2298	A	C2-N3-C4	18.99	120.09	110.60
26	BA	1276	A	C2-N3-C4	18.99	120.09	110.60
1	AA	26	A	N1-C6-N6	-18.99	107.21	118.60
1	AA	448	A	C2-N3-C4	18.99	120.09	110.60
26	BA	2564	A	C2-N3-C4	18.99	120.09	110.60
26	BA	1287	A	C2-N3-C4	18.98	120.09	110.60
26	BA	10	A	C2-N3-C4	18.98	120.09	110.60
26	BA	2052	A	C2-N3-C4	18.98	120.09	110.60
1	AA	782	A	N1-C2-N3	-18.98	119.81	129.30
25	AY	26	A	C2-N3-C4	18.98	120.09	110.60
23	AW	59	A	C2-N3-C4	18.98	120.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	6	A	C2-N3-C4	18.98	120.09	110.60
26	BA	1597	A	C2-N3-C4	18.98	120.09	110.60
26	BA	1664	A	C2-N3-C4	18.98	120.09	110.60
26	BA	1545	A	N1-C2-N3	-18.98	119.81	129.30
1	AA	478	A	C2-N3-C4	18.98	120.09	110.60
1	AA	553	A	C2-N3-C4	18.98	120.09	110.60
26	BA	219	A	C2-N3-C4	18.98	120.09	110.60
26	BA	2211	A	C2-N3-C4	18.98	120.09	110.60
24	AX	14	A	C2-N3-C4	18.97	120.09	110.60
26	BA	131	A	C2-N3-C4	18.97	120.09	110.60
26	BA	933	A	C2-N3-C4	18.97	120.09	110.60
26	BA	2471	A	C2-N3-C4	18.97	120.09	110.60
1	AA	539	A	C2-N3-C4	18.97	120.08	110.60
1	AA	964	A	C2-N3-C4	18.97	120.08	110.60
26	BA	574	A	N1-C6-N6	-18.97	107.22	118.60
26	BA	2887	A	C2-N3-C4	18.97	120.08	110.60
27	BB	78	A	N1-C2-N3	-18.97	119.81	129.30
1	AA	1238	A	N1-C6-N6	-18.97	107.22	118.60
23	AW	73	A	C2-N3-C4	18.97	120.08	110.60
26	BA	909	A	N1-C6-N6	-18.97	107.22	118.60
26	BA	532	A	N1-C2-N3	-18.96	119.82	129.30
26	BA	2823	A	C2-N3-C4	18.96	120.08	110.60
1	AA	320	A	C2-N3-C4	18.96	120.08	110.60
26	BA	144	A	C2-N3-C4	18.96	120.08	110.60
1	AA	787	A	C2-N3-C4	18.96	120.08	110.60
26	BA	84	A	N1-C2-N3	-18.96	119.82	129.30
26	BA	1214	A	N1-C2-N3	-18.96	119.82	129.30
26	BA	1829	A	C2-N3-C4	18.96	120.08	110.60
26	BA	2030	A	C2-N3-C4	18.96	120.08	110.60
1	AA	432	A	C2-N3-C4	18.96	120.08	110.60
1	AA	1176	A	C2-N3-C4	18.96	120.08	110.60
26	BA	71	A	C2-N3-C4	18.96	120.08	110.60
26	BA	727	A	C2-N3-C4	18.95	120.08	110.60
26	BA	2461	A	C2-N3-C4	18.95	120.08	110.60
1	AA	171	A	C2-N3-C4	18.95	120.08	110.60
1	AA	780	A	C2-N3-C4	18.95	120.08	110.60
1	AA	784	A	C2-N3-C4	18.95	120.08	110.60
1	AA	1493	A	C2-N3-C4	18.95	120.08	110.60
23	AW	42	A	N1-C2-N3	-18.95	119.82	129.30
25	AY	26	A	N1-C2-N3	-18.95	119.82	129.30
26	BA	204	A	N1-C2-N3	-18.95	119.82	129.30
26	BA	918	A	N1-C6-N6	-18.95	107.23	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1590	A	N1-C6-N6	-18.95	107.23	118.60
26	BA	2761	A	C2-N3-C4	18.95	120.08	110.60
1	AA	55	A	C2-N3-C4	18.95	120.08	110.60
1	AA	179	A	N1-C6-N6	-18.95	107.23	118.60
23	AW	9	A	C2-N3-C4	18.95	120.07	110.60
26	BA	374	A	C2-N3-C4	18.95	120.07	110.60
26	BA	1046	A	C2-N3-C4	18.95	120.07	110.60
26	BA	2054	A	C2-N3-C4	18.95	120.07	110.60
1	AA	681	A	N1-C6-N6	-18.95	107.23	118.60
26	BA	1155	A	N1-C6-N6	-18.95	107.23	118.60
26	BA	2566	A	N1-C6-N6	-18.95	107.23	118.60
26	BA	2516	A	C2-N3-C4	18.94	120.07	110.60
26	BA	800	A	N1-C2-N3	-18.94	119.83	129.30
26	BA	917	A	C2-N3-C4	18.94	120.07	110.60
1	AA	1363	A	C2-N3-C4	18.94	120.07	110.60
26	BA	1028	A	C2-N3-C4	18.94	120.07	110.60
26	BA	1668	A	N1-C6-N6	-18.94	107.24	118.60
1	AA	53	A	C2-N3-C4	18.94	120.07	110.60
1	AA	243	A	N1-C6-N6	-18.94	107.24	118.60
23	AW	9	A	N1-C6-N6	-18.94	107.24	118.60
26	BA	44	A	C2-N3-C4	18.94	120.07	110.60
26	BA	825	A	C2-N3-C4	18.94	120.07	110.60
26	BA	1057	A	N1-C2-N3	-18.94	119.83	129.30
26	BA	2298	A	N1-C2-N3	-18.94	119.83	129.30
26	BA	2418	A	N1-C2-N3	-18.94	119.83	129.30
1	AA	766	A	C2-N3-C4	18.93	120.07	110.60
1	AA	1227	A	C2-N3-C4	18.93	120.07	110.60
26	BA	181	A	C2-N3-C4	18.93	120.07	110.60
26	BA	330	A	C2-N3-C4	18.93	120.07	110.60
26	BA	2469	A	C2-N3-C4	18.93	120.07	110.60
1	AA	889	A	N1-C2-N3	-18.93	119.83	129.30
27	BB	53	A	C2-N3-C4	18.93	120.07	110.60
1	AA	496	A	C2-N3-C4	18.93	120.06	110.60
1	AA	743	A	C2-N3-C4	18.93	120.07	110.60
26	BA	173	A	C2-N3-C4	18.93	120.07	110.60
26	BA	845	A	C2-N3-C4	18.93	120.07	110.60
26	BA	2761	A	N1-C6-N6	-18.93	107.24	118.60
1	AA	373	A	C2-N3-C4	18.93	120.06	110.60
1	AA	533	A	N1-C6-N6	-18.93	107.24	118.60
1	AA	640	A	C2-N3-C4	18.93	120.06	110.60
26	BA	354	A	N1-C6-N6	-18.93	107.24	118.60
26	BA	2117	A	C2-N3-C4	18.93	120.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	371	A	C2-N3-C4	18.93	120.06	110.60
1	AA	431	A	C2-N3-C4	18.93	120.06	110.60
26	BA	1998	A	C2-N3-C4	18.93	120.06	110.60
26	BA	2225	A	C2-N3-C4	18.93	120.06	110.60
26	BA	2503	A	C2-N3-C4	18.93	120.06	110.60
26	BA	2764	A	N1-C2-N3	-18.93	119.83	129.30
27	BB	115	A	C2-N3-C4	18.93	120.06	110.60
1	AA	182	A	N1-C6-N6	-18.93	107.24	118.60
1	AA	1275	A	C2-N3-C4	18.93	120.06	110.60
26	BA	2705	A	C2-N3-C4	18.93	120.06	110.60
1	AA	309	A	N1-C6-N6	-18.93	107.24	118.60
26	BA	348	A	C2-N3-C4	18.93	120.06	110.60
26	BA	352	A	C2-N3-C4	18.93	120.06	110.60
26	BA	1147	A	N1-C2-N3	-18.93	119.84	129.30
26	BA	1785	A	N1-C2-N3	-18.93	119.84	129.30
1	AA	696	A	C2-N3-C4	18.92	120.06	110.60
24	AX	23	A	C2-N3-C4	18.92	120.06	110.60
26	BA	941	A	C2-N3-C4	18.92	120.06	110.60
26	BA	1937	A	N1-C6-N6	-18.92	107.25	118.60
26	BA	2077	A	C2-N3-C4	18.92	120.06	110.60
26	BA	2868	A	C2-N3-C4	18.92	120.06	110.60
1	AA	223	A	C2-N3-C4	18.92	120.06	110.60
1	AA	228	A	C2-N3-C4	18.92	120.06	110.60
1	AA	768	A	C2-N3-C4	18.92	120.06	110.60
26	BA	38	A	N1-C6-N6	-18.92	107.25	118.60
26	BA	42	A	N1-C2-N3	-18.92	119.84	129.30
26	BA	152	A	C2-N3-C4	18.92	120.06	110.60
26	BA	526	A	C2-N3-C4	18.92	120.06	110.60
26	BA	959	A	C2-N3-C4	18.92	120.06	110.60
26	BA	1268	A	C2-N3-C4	18.92	120.06	110.60
1	AA	182	A	C2-N3-C4	18.92	120.06	110.60
1	AA	412	A	N1-C6-N6	-18.92	107.25	118.60
1	AA	915	A	C2-N3-C4	18.92	120.06	110.60
26	BA	2758	A	C2-N3-C4	18.92	120.06	110.60
1	AA	71	A	C2-N3-C4	18.92	120.06	110.60
26	BA	1384	A	C2-N3-C4	18.92	120.06	110.60
1	AA	1349	A	C2-N3-C4	18.92	120.06	110.60
26	BA	190	A	C2-N3-C4	18.92	120.06	110.60
26	BA	693	A	C2-N3-C4	18.92	120.06	110.60
26	BA	1427	A	N1-C2-N3	-18.92	119.84	129.30
26	BA	1098	A	C2-N3-C4	18.91	120.06	110.60
26	BA	1308	A	C2-N3-C4	18.91	120.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1701	A	C2-N3-C4	18.91	120.06	110.60
26	BA	2009	A	N1-C6-N6	-18.91	107.25	118.60
26	BA	2198	A	C2-N3-C4	18.91	120.06	110.60
1	AA	19	A	C2-N3-C4	18.91	120.06	110.60
1	AA	1044	A	C2-N3-C4	18.91	120.06	110.60
24	AX	41	A	C2-N3-C4	18.91	120.06	110.60
26	BA	878	A	C2-N3-C4	18.91	120.06	110.60
26	BA	1932	A	C2-N3-C4	18.91	120.06	110.60
26	BA	2298	A	N1-C6-N6	-18.91	107.25	118.60
26	BA	877	A	C2-N3-C4	18.91	120.06	110.60
26	BA	1803	A	N1-C6-N6	-18.91	107.25	118.60
1	AA	1251	A	C2-N3-C4	18.91	120.05	110.60
1	AA	1410	A	N1-C6-N6	-18.91	107.25	118.60
26	BA	900	A	C2-N3-C4	18.91	120.05	110.60
1	AA	8	A	C2-N3-C4	18.91	120.05	110.60
1	AA	151	A	N1-C2-N3	-18.91	119.85	129.30
23	AW	41	A	C2-N3-C4	18.91	120.05	110.60
26	BA	480	A	N1-C2-N3	-18.91	119.85	129.30
26	BA	1652	A	N1-C6-N6	-18.91	107.26	118.60
26	BA	1772	A	C2-N3-C4	18.91	120.05	110.60
26	BA	2900	A	C2-N3-C4	18.91	120.05	110.60
1	AA	1311	A	C2-N3-C4	18.91	120.05	110.60
1	AA	1340	A	C2-N3-C4	18.91	120.05	110.60
26	BA	167	A	C2-N3-C4	18.91	120.05	110.60
26	BA	203	A	C2-N3-C4	18.91	120.05	110.60
26	BA	233	A	C2-N3-C4	18.91	120.05	110.60
26	BA	2005	A	N1-C6-N6	-18.91	107.26	118.60
26	BA	2281	A	C2-N3-C4	18.91	120.05	110.60
27	BB	29	A	C2-N3-C4	18.91	120.05	110.60
26	BA	863	A	C2-N3-C4	18.90	120.05	110.60
26	BA	2241	A	C2-N3-C4	18.90	120.05	110.60
26	BA	2835	A	C2-N3-C4	18.90	120.05	110.60
1	AA	914	A	C2-N3-C4	18.90	120.05	110.60
1	AA	1151	A	N1-C6-N6	-18.90	107.26	118.60
26	BA	324	A	C2-N3-C4	18.90	120.05	110.60
26	BA	1668	A	C2-N3-C4	18.90	120.05	110.60
26	BA	1772	A	N1-C6-N6	-18.90	107.26	118.60
26	BA	1773	A	C2-N3-C4	18.90	120.05	110.60
26	BA	2727	A	C2-N3-C4	18.90	120.05	110.60
1	AA	282	A	C2-N3-C4	18.90	120.05	110.60
26	BA	750	A	C2-N3-C4	18.90	120.05	110.60
26	BA	1749	A	C2-N3-C4	18.90	120.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1794	A	C2-N3-C4	18.90	120.05	110.60
26	BA	2117	A	N1-C2-N3	-18.90	119.85	129.30
26	BA	2820	A	C2-N3-C4	18.90	120.05	110.60
1	AA	270	A	C2-N3-C4	18.90	120.05	110.60
1	AA	313	A	C2-N3-C4	18.90	120.05	110.60
1	AA	353	A	C2-N3-C4	18.90	120.05	110.60
1	AA	712	A	C2-N3-C4	18.90	120.05	110.60
1	AA	1534	A	C2-N3-C4	18.90	120.05	110.60
23	AW	42	A	C2-N3-C4	18.90	120.05	110.60
26	BA	1717	A	C2-N3-C4	18.90	120.05	110.60
1	AA	149	A	C2-N3-C4	18.90	120.05	110.60
1	AA	1428	A	C2-N3-C4	18.90	120.05	110.60
26	BA	1084	A	C2-N3-C4	18.90	120.05	110.60
1	AA	452	A	C2-N3-C4	18.90	120.05	110.60
1	AA	460	A	C2-N3-C4	18.90	120.05	110.60
1	AA	694	A	C2-N3-C4	18.90	120.05	110.60
1	AA	1082	A	C2-N3-C4	18.90	120.05	110.60
1	AA	1360	A	C2-N3-C4	18.90	120.05	110.60
26	BA	2590	A	N1-C6-N6	-18.90	107.26	118.60
1	AA	621	A	C2-N3-C4	18.89	120.05	110.60
1	AA	1499	A	C2-N3-C4	18.89	120.05	110.60
26	BA	1919	A	N1-C2-N3	-18.89	119.85	129.30
26	BA	2070	A	N1-C6-N6	-18.89	107.26	118.60
1	AA	60	A	N1-C2-N3	-18.89	119.85	129.30
1	AA	704	A	C2-N3-C4	18.89	120.05	110.60
1	AA	706	A	C2-N3-C4	18.89	120.05	110.60
26	BA	460	A	N1-C6-N6	-18.89	107.26	118.60
26	BA	1302	A	C2-N3-C4	18.89	120.05	110.60
26	BA	1427	A	C2-N3-C4	18.89	120.05	110.60
26	BA	2764	A	C2-N3-C4	18.89	120.05	110.60
1	AA	411	A	C2-N3-C4	18.89	120.05	110.60
1	AA	1333	A	N1-C2-N3	-18.89	119.85	129.30
26	BA	1548	A	C2-N3-C4	18.89	120.05	110.60
1	AA	72	A	C2-N3-C4	18.89	120.05	110.60
1	AA	393	A	N1-C2-N3	-18.89	119.86	129.30
1	AA	1169	A	C2-N3-C4	18.89	120.05	110.60
1	AA	1480	A	C2-N3-C4	18.89	120.05	110.60
23	AW	23	A	C2-N3-C4	18.89	120.05	110.60
26	BA	309	A	C2-N3-C4	18.89	120.05	110.60
26	BA	849	A	N1-C6-N6	-18.89	107.27	118.60
26	BA	1054	A	C2-N3-C4	18.89	120.05	110.60
26	BA	1286	A	C2-N3-C4	18.89	120.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2169	A	C2-N3-C4	18.89	120.05	110.60
26	BA	2327	A	C2-N3-C4	18.89	120.05	110.60
27	BB	34	A	N1-C2-N3	-18.89	119.86	129.30
24	AX	24	A	C2-N3-C4	18.89	120.04	110.60
26	BA	197	A	C2-N3-C4	18.89	120.04	110.60
26	BA	262	A	C2-N3-C4	18.89	120.05	110.60
26	BA	1960	A	N1-C6-N6	-18.89	107.27	118.60
26	BA	2388	A	C2-N3-C4	18.89	120.04	110.60
24	AX	26	A	C2-N3-C4	18.89	120.04	110.60
26	BA	504	A	C2-N3-C4	18.89	120.04	110.60
26	BA	644	A	C2-N3-C4	18.89	120.04	110.60
26	BA	1010	A	C2-N3-C4	18.89	120.04	110.60
26	BA	1264	A	C2-N3-C4	18.89	120.04	110.60
26	BA	1308	A	N1-C6-N6	-18.89	107.27	118.60
26	BA	1755	A	N1-C6-N6	-18.89	107.27	118.60
26	BA	1048	A	C2-N3-C4	18.88	120.04	110.60
1	AA	411	A	N1-C2-N3	-18.88	119.86	129.30
1	AA	1269	A	C2-N3-C4	18.88	120.04	110.60
25	AY	69	A	C2-N3-C4	18.88	120.04	110.60
26	BA	460	A	C2-N3-C4	18.88	120.04	110.60
26	BA	1634	A	C2-N3-C4	18.88	120.04	110.60
26	BA	2163	A	C2-N3-C4	18.88	120.04	110.60
1	AA	131	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	642	A	C2-N3-C4	18.88	120.04	110.60
1	AA	1248	A	N1-C6-N6	-18.88	107.27	118.60
26	BA	1214	A	N1-C6-N6	-18.88	107.27	118.60
26	BA	2513	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	44	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	167	A	C2-N3-C4	18.88	120.04	110.60
1	AA	189	A	C2-N3-C4	18.88	120.04	110.60
1	AA	749	A	C2-N3-C4	18.88	120.04	110.60
1	AA	938	A	C2-N3-C4	18.88	120.04	110.60
1	AA	1368	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	1429	A	C2-N3-C4	18.88	120.04	110.60
26	BA	142	A	C2-N3-C4	18.88	120.04	110.60
26	BA	1515	A	C2-N3-C4	18.88	120.04	110.60
26	BA	2154	A	N1-C2-N3	-18.88	119.86	129.30
26	BA	2450	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	199	A	C2-N3-C4	18.88	120.04	110.60
1	AA	1254	A	C2-N3-C4	18.88	120.04	110.60
26	BA	241	A	N1-C2-N3	-18.88	119.86	129.30
26	BA	241	A	N1-C6-N6	-18.88	107.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1014	A	N1-C2-N3	-18.88	119.86	129.30
26	BA	2872	A	C2-N3-C4	18.88	120.04	110.60
1	AA	452	A	N1-C2-N3	-18.88	119.86	129.30
25	AY	66	A	C2-N3-C4	18.88	120.04	110.60
26	BA	1787	A	C2-N3-C4	18.88	120.04	110.60
26	BA	2225	A	N1-C2-N3	-18.88	119.86	129.30
26	BA	2741	A	N1-C2-N3	-18.88	119.86	129.30
26	BA	1127	A	C2-N3-C4	18.88	120.04	110.60
1	AA	915	A	N1-C6-N6	-18.87	107.28	118.60
26	BA	191	A	C2-N3-C4	18.87	120.04	110.60
26	BA	582	A	C2-N3-C4	18.87	120.04	110.60
26	BA	689	A	C2-N3-C4	18.87	120.04	110.60
26	BA	1169	A	C2-N3-C4	18.87	120.04	110.60
26	BA	1502	A	C2-N3-C4	18.87	120.04	110.60
26	BA	2173	A	C2-N3-C4	18.87	120.04	110.60
1	AA	65	A	C2-N3-C4	18.87	120.04	110.60
26	BA	980	A	C2-N3-C4	18.87	120.04	110.60
26	BA	2101	A	C2-N3-C4	18.87	120.04	110.60
1	AA	1105	A	C2-N3-C4	18.87	120.04	110.60
26	BA	231	A	C2-N3-C4	18.87	120.04	110.60
26	BA	794	A	C2-N3-C4	18.87	120.03	110.60
26	BA	1262	A	N1-C6-N6	-18.87	107.28	118.60
26	BA	2199	A	C2-N3-C4	18.87	120.03	110.60
26	BA	2407	A	C2-N3-C4	18.87	120.03	110.60
26	BA	2741	A	C2-N3-C4	18.87	120.04	110.60
1	AA	909	A	C2-N3-C4	18.87	120.03	110.60
26	BA	2757	A	C2-N3-C4	18.87	120.03	110.60
26	BA	1632	A	C2-N3-C4	18.87	120.03	110.60
1	AA	412	A	N1-C2-N3	-18.87	119.87	129.30
26	BA	1618	A	C2-N3-C4	18.87	120.03	110.60
27	BB	39	A	C2-N3-C4	18.87	120.03	110.60
1	AA	441	A	C2-N3-C4	18.86	120.03	110.60
1	AA	1102	A	C2-N3-C4	18.86	120.03	110.60
26	BA	368	A	C2-N3-C4	18.86	120.03	110.60
26	BA	1307	A	C2-N3-C4	18.86	120.03	110.60
26	BA	2322	A	N1-C2-N3	-18.86	119.87	129.30
26	BA	2381	A	C2-N3-C4	18.86	120.03	110.60
26	BA	2435	A	C2-N3-C4	18.86	120.03	110.60
26	BA	1419	A	N1-C2-N3	-18.86	119.87	129.30
26	BA	2314	A	C2-N3-C4	18.86	120.03	110.60
1	AA	327	A	N1-C2-N3	-18.86	119.87	129.30
1	AA	495	A	C2-N3-C4	18.86	120.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	958	A	C2-N3-C4	18.86	120.03	110.60
26	BA	111	A	N1-C6-N6	-18.86	107.28	118.60
26	BA	244	A	C2-N3-C4	18.86	120.03	110.60
26	BA	788	A	C2-N3-C4	18.86	120.03	110.60
26	BA	802	A	N1-C6-N6	-18.86	107.28	118.60
26	BA	979	A	C2-N3-C4	18.86	120.03	110.60
26	BA	1069	A	C2-N3-C4	18.86	120.03	110.60
26	BA	2033	A	N1-C2-N3	-18.86	119.87	129.30
26	BA	2381	A	N1-C6-N6	-18.86	107.28	118.60
26	BA	2589	A	N1-C2-N3	-18.86	119.87	129.30
26	BA	2829	A	C2-N3-C4	18.86	120.03	110.60
26	BA	6	A	C2-N3-C4	18.86	120.03	110.60
26	BA	111	A	C2-N3-C4	18.86	120.03	110.60
26	BA	990	A	N1-C2-N3	-18.86	119.87	129.30
26	BA	1419	A	C2-N3-C4	18.86	120.03	110.60
26	BA	1689	A	C2-N3-C4	18.86	120.03	110.60
26	BA	2377	A	C2-N3-C4	18.86	120.03	110.60
1	AA	1507	A	C2-N3-C4	18.86	120.03	110.60
26	BA	792	A	C2-N3-C4	18.86	120.03	110.60
26	BA	2247	A	N1-C2-N3	-18.86	119.87	129.30
1	AA	119	A	C2-N3-C4	18.86	120.03	110.60
1	AA	160	A	C2-N3-C4	18.86	120.03	110.60
1	AA	600	A	C2-N3-C4	18.86	120.03	110.60
26	BA	502	A	C2-N3-C4	18.86	120.03	110.60
26	BA	529	A	N1-C6-N6	-18.86	107.29	118.60
26	BA	661	A	C2-N3-C4	18.86	120.03	110.60
26	BA	1342	A	C2-N3-C4	18.86	120.03	110.60
26	BA	1579	A	C2-N3-C4	18.86	120.03	110.60
26	BA	1665	A	C2-N3-C4	18.86	120.03	110.60
26	BA	1786	A	C2-N3-C4	18.86	120.03	110.60
26	BA	1805	A	C2-N3-C4	18.86	120.03	110.60
26	BA	2031	A	C2-N3-C4	18.86	120.03	110.60
1	AA	1000	A	N1-C6-N6	-18.86	107.29	118.60
26	BA	1544	A	C2-N3-C4	18.86	120.03	110.60
1	AA	120	A	C2-N3-C4	18.85	120.03	110.60
26	BA	522	A	C2-N3-C4	18.85	120.03	110.60
26	BA	1001	A	N1-C6-N6	-18.85	107.29	118.60
26	BA	1272	A	C2-N3-C4	18.85	120.03	110.60
26	BA	2284	A	C2-N3-C4	18.85	120.03	110.60
26	BA	2386	A	C2-N3-C4	18.85	120.03	110.60
26	BA	2590	A	C2-N3-C4	18.85	120.03	110.60
26	BA	2700	A	C2-N3-C4	18.85	120.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2879	A	C2-N3-C4	18.85	120.03	110.60
27	BB	57	A	C2-N3-C4	18.85	120.03	110.60
1	AA	665	A	C2-N3-C4	18.85	120.03	110.60
26	BA	608	A	C2-N3-C4	18.85	120.03	110.60
26	BA	1336	A	C2-N3-C4	18.85	120.03	110.60
26	BA	1593	A	C2-N3-C4	18.85	120.03	110.60
26	BA	2835	A	N1-C2-N3	-18.85	119.87	129.30
1	AA	363	A	C2-N3-C4	18.85	120.03	110.60
1	AA	1311	A	N1-C6-N6	-18.85	107.29	118.60
26	BA	320	A	C2-N3-C4	18.85	120.03	110.60
26	BA	324	A	N1-C2-N3	-18.85	119.88	129.30
26	BA	825	A	N1-C6-N6	-18.85	107.29	118.60
26	BA	1596	A	C2-N3-C4	18.85	120.03	110.60
26	BA	2792	A	C2-N3-C4	18.85	120.03	110.60
26	BA	2850	A	C2-N3-C4	18.85	120.03	110.60
26	BA	149	A	C2-N3-C4	18.85	120.03	110.60
26	BA	675	A	C2-N3-C4	18.85	120.03	110.60
1	AA	131	A	C2-N3-C4	18.85	120.02	110.60
1	AA	412	A	C2-N3-C4	18.85	120.02	110.60
24	AX	3	A	C2-N3-C4	18.85	120.02	110.60
25	AY	14	A	C2-N3-C4	18.85	120.02	110.60
26	BA	84	A	C2-N3-C4	18.85	120.02	110.60
26	BA	95	A	C2-N3-C4	18.85	120.02	110.60
26	BA	1274	A	C2-N3-C4	18.85	120.02	110.60
26	BA	1366	A	C2-N3-C4	18.85	120.02	110.60
26	BA	1746	A	C2-N3-C4	18.85	120.02	110.60
26	BA	1847	A	C2-N3-C4	18.85	120.02	110.60
26	BA	2411	A	C2-N3-C4	18.85	120.02	110.60
1	AA	572	A	C2-N3-C4	18.85	120.02	110.60
1	AA	746	A	C2-N3-C4	18.85	120.02	110.60
26	BA	1470	A	C2-N3-C4	18.85	120.02	110.60
26	BA	2388	A	N1-C2-N3	-18.85	119.88	129.30
1	AA	26	A	C2-N3-C4	18.84	120.02	110.60
1	AA	181	A	C2-N3-C4	18.84	120.02	110.60
1	AA	432	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	1016	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1456	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1476	A	C2-N3-C4	18.84	120.02	110.60
26	BA	28	A	C2-N3-C4	18.84	120.02	110.60
26	BA	146	A	C2-N3-C4	18.84	120.02	110.60
26	BA	199	A	C2-N3-C4	18.84	120.02	110.60
26	BA	223	A	C2-N3-C4	18.84	120.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	391	A	C2-N3-C4	18.84	120.02	110.60
26	BA	621	A	N1-C2-N3	-18.84	119.88	129.30
26	BA	1304	A	N1-C6-N6	-18.84	107.29	118.60
26	BA	1608	A	C2-N3-C4	18.84	120.02	110.60
26	BA	1853	A	C2-N3-C4	18.84	120.02	110.60
26	BA	2158	A	C2-N3-C4	18.84	120.02	110.60
26	BA	2453	A	C2-N3-C4	18.84	120.02	110.60
26	BA	2476	A	C2-N3-C4	18.84	120.02	110.60
1	AA	389	A	N1-C2-N3	-18.84	119.88	129.30
26	BA	449	A	C2-N3-C4	18.84	120.02	110.60
26	BA	2108	A	N1-C6-N6	-18.84	107.29	118.60
26	BA	2346	A	C2-N3-C4	18.84	120.02	110.60
26	BA	2634	A	C2-N3-C4	18.84	120.02	110.60
1	AA	16	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	78	A	C2-N3-C4	18.84	120.02	110.60
1	AA	482	A	C2-N3-C4	18.84	120.02	110.60
1	AA	583	A	C2-N3-C4	18.84	120.02	110.60
1	AA	629	A	C2-N3-C4	18.84	120.02	110.60
1	AA	807	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1339	A	C2-N3-C4	18.84	120.02	110.60
26	BA	222	A	C2-N3-C4	18.84	120.02	110.60
26	BA	457	A	N1-C2-N3	-18.84	119.88	129.30
26	BA	572	A	C2-N3-C4	18.84	120.02	110.60
26	BA	631	A	C2-N3-C4	18.84	120.02	110.60
26	BA	983	A	C2-N3-C4	18.84	120.02	110.60
26	BA	2388	A	N1-C6-N6	-18.84	107.30	118.60
26	BA	2899	A	C2-N3-C4	18.84	120.02	110.60
1	AA	327	A	C2-N3-C4	18.84	120.02	110.60
1	AA	825	A	N1-C6-N6	-18.84	107.30	118.60
1	AA	1408	A	C2-N3-C4	18.84	120.02	110.60
26	BA	207	A	C2-N3-C4	18.84	120.02	110.60
26	BA	218	A	C2-N3-C4	18.84	120.02	110.60
26	BA	735	A	C2-N3-C4	18.84	120.02	110.60
26	BA	1772	A	N1-C2-N3	-18.84	119.88	129.30
26	BA	2665	A	C2-N3-C4	18.84	120.02	110.60
1	AA	673	A	C2-N3-C4	18.84	120.02	110.60
1	AA	766	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	1503	A	C2-N3-C4	18.84	120.02	110.60
23	AW	41	A	N1-C6-N6	-18.84	107.30	118.60
25	AY	58	A	C2-N3-C4	18.84	120.02	110.60
26	BA	332	A	C2-N3-C4	18.84	120.02	110.60
26	BA	1953	A	N1-C2-N3	-18.84	119.88	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2660	A	C2-N3-C4	18.84	120.02	110.60
1	AA	382	A	C2-N3-C4	18.84	120.02	110.60
1	AA	983	A	N1-C2-N3	-18.84	119.88	129.30
26	BA	2090	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	26	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	32	A	C2-N3-C4	18.84	120.02	110.60
1	AA	456	A	C2-N3-C4	18.84	120.02	110.60
1	AA	889	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1446	A	C2-N3-C4	18.84	120.02	110.60
26	BA	14	A	C2-N3-C4	18.84	120.02	110.60
26	BA	176	A	C2-N3-C4	18.84	120.02	110.60
26	BA	401	A	C2-N3-C4	18.84	120.02	110.60
26	BA	429	A	C2-N3-C4	18.84	120.02	110.60
26	BA	2241	A	N1-C6-N6	-18.84	107.30	118.60
26	BA	2418	A	C2-N3-C4	18.84	120.02	110.60
26	BA	2439	A	C2-N3-C4	18.84	120.02	110.60
26	BA	2564	A	N1-C2-N3	-18.84	119.88	129.30
26	BA	2882	A	C2-N3-C4	18.84	120.02	110.60
27	BB	104	A	C2-N3-C4	18.84	120.02	110.60
27	BB	119	A	C2-N3-C4	18.84	120.02	110.60
26	BA	508	A	C2-N3-C4	18.83	120.02	110.60
26	BA	718	A	C2-N3-C4	18.83	120.02	110.60
26	BA	1650	A	C2-N3-C4	18.83	120.02	110.60
26	BA	2534	A	C2-N3-C4	18.83	120.02	110.60
26	BA	2541	A	C2-N3-C4	18.83	120.02	110.60
1	AA	533	A	C2-N3-C4	18.83	120.02	110.60
1	AA	831	A	C2-N3-C4	18.83	120.02	110.60
1	AA	1289	A	N1-C6-N6	-18.83	107.30	118.60
26	BA	270	A	C2-N3-C4	18.83	120.02	110.60
26	BA	423	A	C2-N3-C4	18.83	120.02	110.60
26	BA	428	A	C2-N3-C4	18.83	120.02	110.60
26	BA	910	A	N1-C6-N6	-18.83	107.30	118.60
26	BA	1226	A	C2-N3-C4	18.83	120.02	110.60
26	BA	1254	A	C2-N3-C4	18.83	120.02	110.60
26	BA	2333	A	C2-N3-C4	18.83	120.02	110.60
26	BA	2426	A	C2-N3-C4	18.83	120.02	110.60
26	BA	2587	A	C2-N3-C4	18.83	120.02	110.60
26	BA	2632	A	N1-C6-N6	-18.83	107.30	118.60
1	AA	560	A	C2-N3-C4	18.83	120.02	110.60
1	AA	573	A	C2-N3-C4	18.83	120.02	110.60
26	BA	1630	A	N1-C2-N3	-18.83	119.88	129.30
26	BA	2037	A	N1-C2-N3	-18.83	119.88	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2459	A	C2-N3-C4	18.83	120.02	110.60
1	AA	414	A	C2-N3-C4	18.83	120.02	110.60
1	AA	900	A	C2-N3-C4	18.83	120.01	110.60
26	BA	497	A	C2-N3-C4	18.83	120.02	110.60
26	BA	529	A	N1-C2-N3	-18.83	119.89	129.30
26	BA	699	A	C2-N3-C4	18.83	120.02	110.60
26	BA	1040	A	C2-N3-C4	18.83	120.02	110.60
26	BA	1040	A	N1-C2-N3	-18.83	119.89	129.30
26	BA	1067	A	C2-N3-C4	18.83	120.02	110.60
26	BA	1419	A	N1-C6-N6	-18.83	107.30	118.60
26	BA	1802	A	C2-N3-C4	18.83	120.02	110.60
26	BA	2009	A	N1-C2-N3	-18.83	119.89	129.30
26	BA	2425	A	C2-N3-C4	18.83	120.02	110.60
26	BA	2468	A	C2-N3-C4	18.83	120.02	110.60
26	BA	2478	A	C2-N3-C4	18.83	120.02	110.60
1	AA	44	A	C2-N3-C4	18.83	120.01	110.60
1	AA	236	A	C2-N3-C4	18.83	120.01	110.60
1	AA	630	A	C2-N3-C4	18.83	120.01	110.60
1	AA	675	A	C2-N3-C4	18.83	120.01	110.60
1	AA	1350	A	C2-N3-C4	18.83	120.01	110.60
26	BA	125	A	C2-N3-C4	18.83	120.01	110.60
26	BA	181	A	N1-C2-N3	-18.83	119.89	129.30
26	BA	472	A	C2-N3-C4	18.83	120.01	110.60
26	BA	599	A	C2-N3-C4	18.83	120.01	110.60
26	BA	1050	A	C2-N3-C4	18.83	120.01	110.60
26	BA	1672	A	C2-N3-C4	18.83	120.01	110.60
26	BA	1916	A	C2-N3-C4	18.83	120.01	110.60
26	BA	2736	A	N1-C6-N6	-18.83	107.30	118.60
1	AA	777	A	C2-N3-C4	18.83	120.01	110.60
1	AA	1179	A	C2-N3-C4	18.83	120.01	110.60
25	AY	38	A	C2-N3-C4	18.83	120.01	110.60
26	BA	182	A	N1-C6-N6	-18.83	107.30	118.60
26	BA	1569	A	C2-N3-C4	18.83	120.01	110.60
26	BA	1889	A	C2-N3-C4	18.83	120.01	110.60
26	BA	2042	A	C2-N3-C4	18.83	120.01	110.60
1	AA	1204	A	C2-N3-C4	18.82	120.01	110.60
26	BA	42	A	N1-C6-N6	-18.82	107.31	118.60
26	BA	155	A	C2-N3-C4	18.82	120.01	110.60
26	BA	221	A	C2-N3-C4	18.82	120.01	110.60
26	BA	668	A	N1-C6-N6	-18.82	107.31	118.60
26	BA	905	A	N1-C2-N3	-18.82	119.89	129.30
26	BA	1246	A	C2-N3-C4	18.82	120.01	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2530	A	C2-N3-C4	18.82	120.01	110.60
26	BA	2873	A	C2-N3-C4	18.82	120.01	110.60
26	BA	2893	A	C2-N3-C4	18.82	120.01	110.60
26	BA	1069	A	N1-C2-N3	-18.82	119.89	129.30
26	BA	1713	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	498	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	635	A	C2-N3-C4	18.82	120.01	110.60
1	AA	946	A	C2-N3-C4	18.82	120.01	110.60
1	AA	1394	A	N1-C2-N3	-18.82	119.89	129.30
22	AV	22	A	C2-N3-C4	18.82	120.01	110.60
24	AX	58	A	C2-N3-C4	18.82	120.01	110.60
25	AY	21	A	C2-N3-C4	18.82	120.01	110.60
25	AY	41	A	C2-N3-C4	18.82	120.01	110.60
26	BA	103	A	C2-N3-C4	18.82	120.01	110.60
26	BA	244	A	N1-C6-N6	-18.82	107.31	118.60
26	BA	602	A	C2-N3-C4	18.82	120.01	110.60
26	BA	706	A	C2-N3-C4	18.82	120.01	110.60
26	BA	742	A	C2-N3-C4	18.82	120.01	110.60
26	BA	1144	A	C2-N3-C4	18.82	120.01	110.60
26	BA	1403	A	C2-N3-C4	18.82	120.01	110.60
26	BA	1453	A	C2-N3-C4	18.82	120.01	110.60
26	BA	1783	A	C2-N3-C4	18.82	120.01	110.60
26	BA	1885	A	C2-N3-C4	18.82	120.01	110.60
26	BA	2095	A	C2-N3-C4	18.82	120.01	110.60
26	BA	2478	A	N1-C2-N3	-18.82	119.89	129.30
26	BA	2837	A	C2-N3-C4	18.82	120.01	110.60
1	AA	767	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	1346	A	C2-N3-C4	18.82	120.01	110.60
26	BA	64	A	C2-N3-C4	18.82	120.01	110.60
26	BA	226	A	C2-N3-C4	18.82	120.01	110.60
26	BA	1858	A	C2-N3-C4	18.82	120.01	110.60
1	AA	131	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	253	A	N1-C6-N6	-18.82	107.31	118.60
1	AA	325	A	C2-N3-C4	18.82	120.01	110.60
1	AA	909	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	1410	A	N1-C2-N3	-18.82	119.89	129.30
26	BA	265	A	C2-N3-C4	18.82	120.01	110.60
26	BA	460	A	N1-C2-N3	-18.82	119.89	129.30
26	BA	501	A	C2-N3-C4	18.82	120.01	110.60
26	BA	1304	A	C2-N3-C4	18.82	120.01	110.60
26	BA	2566	A	N1-C2-N3	-18.82	119.89	129.30
26	BA	2741	A	N1-C6-N6	-18.82	107.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2749	A	C2-N3-C4	18.82	120.01	110.60
25	AY	73	A	C2-N3-C4	18.82	120.01	110.60
26	BA	478	A	C2-N3-C4	18.82	120.01	110.60
26	BA	866	A	C2-N3-C4	18.82	120.01	110.60
26	BA	943	A	C2-N3-C4	18.82	120.01	110.60
26	BA	2335	A	C2-N3-C4	18.82	120.01	110.60
26	BA	2757	A	N1-C6-N6	-18.82	107.31	118.60
1	AA	303	A	C2-N3-C4	18.82	120.01	110.60
1	AA	344	A	C2-N3-C4	18.82	120.01	110.60
1	AA	415	A	C2-N3-C4	18.82	120.01	110.60
1	AA	802	A	C2-N3-C4	18.82	120.01	110.60
1	AA	1171	A	C2-N3-C4	18.82	120.01	110.60
22	AV	20	A	C2-N3-C4	18.82	120.01	110.60
26	BA	470	A	C2-N3-C4	18.82	120.01	110.60
26	BA	637	A	C2-N3-C4	18.82	120.01	110.60
26	BA	896	A	C2-N3-C4	18.82	120.01	110.60
26	BA	2503	A	N1-C2-N3	-18.82	119.89	129.30
26	BA	2868	A	N1-C2-N3	-18.82	119.89	129.30
26	BA	2868	A	N1-C6-N6	-18.82	107.31	118.60
1	AA	1219	A	C2-N3-C4	18.81	120.01	110.60
1	AA	1248	A	C2-N3-C4	18.81	120.01	110.60
26	BA	118	A	C2-N3-C4	18.81	120.01	110.60
26	BA	346	A	C2-N3-C4	18.81	120.01	110.60
26	BA	1090	A	C2-N3-C4	18.81	120.01	110.60
26	BA	1668	A	N1-C2-N3	-18.81	119.89	129.30
26	BA	1784	A	N1-C2-N3	-18.81	119.89	129.30
26	BA	2711	A	C2-N3-C4	18.81	120.01	110.60
1	AA	129	A	C2-N3-C4	18.81	120.01	110.60
1	AA	195	A	C2-N3-C4	18.81	120.01	110.60
1	AA	1196	A	C2-N3-C4	18.81	120.01	110.60
1	AA	1275	A	N1-C2-N3	-18.81	119.89	129.30
23	AW	21	A	C2-N3-C4	18.81	120.01	110.60
26	BA	165	A	C2-N3-C4	18.81	120.01	110.60
26	BA	804	A	C2-N3-C4	18.81	120.01	110.60
26	BA	1413	A	C2-N3-C4	18.81	120.01	110.60
26	BA	1871	A	C2-N3-C4	18.81	120.01	110.60
26	BA	2088	A	C2-N3-C4	18.81	120.01	110.60
26	BA	2725	A	C2-N3-C4	18.81	120.01	110.60
1	AA	825	A	C2-N3-C4	18.81	120.00	110.60
26	BA	910	A	N1-C2-N3	-18.81	119.89	129.30
26	BA	1000	A	N1-C6-N6	-18.81	107.31	118.60
26	BA	1126	A	C2-N3-C4	18.81	120.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1165	A	N1-C2-N3	-18.81	119.89	129.30
26	BA	1265	A	C2-N3-C4	18.81	120.00	110.60
26	BA	1952	A	C2-N3-C4	18.81	120.00	110.60
1	AA	648	A	C2-N3-C4	18.81	120.00	110.60
1	AA	1368	A	C2-N3-C4	18.81	120.00	110.60
1	AA	1433	A	C2-N3-C4	18.81	120.00	110.60
23	AW	69	A	C2-N3-C4	18.81	120.00	110.60
23	AW	76	A	C2-N3-C4	18.81	120.00	110.60
25	AY	23	A	C2-N3-C4	18.81	120.00	110.60
26	BA	362	A	N1-C2-N3	-18.81	119.89	129.30
26	BA	454	A	N1-C2-N3	-18.81	119.89	129.30
26	BA	627	A	C2-N3-C4	18.81	120.00	110.60
26	BA	783	A	C2-N3-C4	18.81	120.00	110.60
26	BA	861	A	C2-N3-C4	18.81	120.00	110.60
26	BA	1194	A	C2-N3-C4	18.81	120.00	110.60
26	BA	1204	A	N1-C2-N3	-18.81	119.89	129.30
26	BA	1785	A	C2-N3-C4	18.81	120.00	110.60
26	BA	2005	A	C2-N3-C4	18.81	120.00	110.60
26	BA	2059	A	C2-N3-C4	18.81	120.00	110.60
26	BA	2733	A	C2-N3-C4	18.81	120.00	110.60
26	BA	2778	A	C2-N3-C4	18.81	120.00	110.60
1	AA	179	A	C2-N3-C4	18.81	120.00	110.60
1	AA	749	A	N1-C6-N6	-18.81	107.31	118.60
26	BA	342	A	C2-N3-C4	18.81	120.00	110.60
26	BA	1204	A	C2-N3-C4	18.81	120.00	110.60
26	BA	1901	A	N1-C2-N3	-18.81	119.90	129.30
26	BA	2135	A	C2-N3-C4	18.81	120.00	110.60
26	BA	2821	A	C2-N3-C4	18.81	120.00	110.60
1	AA	1261	A	C2-N3-C4	18.81	120.00	110.60
22	AV	19	A	C2-N3-C4	18.81	120.00	110.60
26	BA	38	A	C2-N3-C4	18.81	120.00	110.60
26	BA	354	A	N1-C2-N3	-18.81	119.90	129.30
26	BA	833	A	C2-N3-C4	18.81	120.00	110.60
26	BA	1354	A	C2-N3-C4	18.81	120.00	110.60
26	BA	1522	A	N1-C2-N3	-18.81	119.90	129.30
26	BA	2184	A	C2-N3-C4	18.81	120.00	110.60
26	BA	2810	A	C2-N3-C4	18.81	120.00	110.60
1	AA	655	A	C2-N3-C4	18.80	120.00	110.60
1	AA	949	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1146	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1257	A	C2-N3-C4	18.80	120.00	110.60
26	BA	155	A	N1-C6-N6	-18.80	107.32	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	730	A	C2-N3-C4	18.80	120.00	110.60
26	BA	849	A	C2-N3-C4	18.80	120.00	110.60
26	BA	947	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	1057	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1265	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	1286	A	N1-C6-N6	-18.80	107.32	118.60
1	AA	192	A	C2-N3-C4	18.80	120.00	110.60
1	AA	309	A	C2-N3-C4	18.80	120.00	110.60
1	AA	864	A	C2-N3-C4	18.80	120.00	110.60
22	AV	15	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	800	A	N1-C6-N6	-18.80	107.32	118.60
26	BA	1367	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1912	A	C2-N3-C4	18.80	120.00	110.60
26	BA	2119	A	C2-N3-C4	18.80	120.00	110.60
26	BA	2134	A	C2-N3-C4	18.80	120.00	110.60
1	AA	510	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1080	A	C2-N3-C4	18.80	120.00	110.60
26	BA	936	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1308	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	1665	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	33	A	C2-N3-C4	18.80	120.00	110.60
1	AA	129	A	N1-C6-N6	-18.80	107.32	118.60
1	AA	338	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	499	A	N1-C6-N6	-18.80	107.32	118.60
1	AA	609	A	C2-N3-C4	18.80	120.00	110.60
1	AA	718	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1093	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1394	A	C2-N3-C4	18.80	120.00	110.60
26	BA	156	A	C2-N3-C4	18.80	120.00	110.60
26	BA	165	A	N1-C6-N6	-18.80	107.32	118.60
26	BA	347	A	C2-N3-C4	18.80	120.00	110.60
26	BA	529	A	C2-N3-C4	18.80	120.00	110.60
26	BA	722	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1073	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1096	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1494	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1593	A	N1-C6-N6	-18.80	107.32	118.60
26	BA	1609	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1801	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1912	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	1916	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	182	A	N1-C2-N3	-18.80	119.90	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	685	A	C2-N3-C4	18.80	120.00	110.60
26	BA	802	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	1937	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	1938	A	C2-N3-C4	18.80	120.00	110.60
26	BA	2478	A	N1-C6-N6	-18.80	107.32	118.60
1	AA	81	A	C2-N3-C4	18.80	120.00	110.60
1	AA	792	A	C2-N3-C4	18.80	120.00	110.60
1	AA	906	A	C2-N3-C4	18.80	120.00	110.60
1	AA	914	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	1204	A	N1-C6-N6	-18.80	107.32	118.60
1	AA	1377	A	C2-N3-C4	18.80	120.00	110.60
26	BA	279	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	480	A	N1-C6-N6	-18.80	107.32	118.60
26	BA	616	A	C2-N3-C4	18.80	120.00	110.60
26	BA	960	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1000	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	1373	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1749	A	N1-C6-N6	-18.80	107.32	118.60
26	BA	2126	A	C2-N3-C4	18.80	120.00	110.60
26	BA	2176	A	N1-C6-N6	-18.80	107.32	118.60
27	BB	94	A	C2-N3-C4	18.80	120.00	110.60
27	BB	99	A	C2-N3-C4	18.80	120.00	110.60
1	AA	430	A	C2-N3-C4	18.80	120.00	110.60
1	AA	523	A	C2-N3-C4	18.80	120.00	110.60
1	AA	535	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	483	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1165	A	N1-C6-N6	-18.80	107.32	118.60
26	BA	1328	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1678	A	C2-N3-C4	18.80	120.00	110.60
26	BA	1794	A	N1-C2-N3	-18.80	119.90	129.30
26	BA	1866	A	C2-N3-C4	18.80	120.00	110.60
26	BA	2052	A	N1-C2-N3	-18.80	119.90	129.30
27	BB	101	A	C2-N3-C4	18.80	120.00	110.60
1	AA	663	A	C2-N3-C4	18.79	120.00	110.60
1	AA	915	A	N1-C2-N3	-18.79	119.90	129.30
1	AA	1197	A	C2-N3-C4	18.79	120.00	110.60
1	AA	1319	A	C2-N3-C4	18.79	120.00	110.60
26	BA	1503	A	C2-N3-C4	18.79	120.00	110.60
26	BA	2071	A	N1-C2-N3	-18.79	119.90	129.30
1	AA	802	A	N1-C2-N3	-18.79	119.90	129.30
1	AA	1019	A	C2-N3-C4	18.79	120.00	110.60
1	AA	1042	A	C2-N3-C4	18.79	120.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1418	A	C2-N3-C4	18.79	120.00	110.60
1	AA	1430	A	C2-N3-C4	18.79	120.00	110.60
1	AA	1493	A	N1-C2-N3	-18.79	119.90	129.30
26	BA	89	A	C2-N3-C4	18.79	120.00	110.60
26	BA	439	A	C2-N3-C4	18.79	120.00	110.60
26	BA	1754	A	C2-N3-C4	18.79	120.00	110.60
26	BA	1960	A	C2-N3-C4	18.79	120.00	110.60
26	BA	1978	A	C2-N3-C4	18.79	120.00	110.60
26	BA	2736	A	C2-N3-C4	18.79	120.00	110.60
26	BA	2856	A	C2-N3-C4	18.79	120.00	110.60
1	AA	130	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	172	A	N1-C6-N6	-18.79	107.33	118.60
1	AA	1167	A	N1-C2-N3	-18.79	119.91	129.30
26	BA	666	A	C2-N3-C4	18.79	120.00	110.60
26	BA	861	A	N1-C6-N6	-18.79	107.33	118.60
26	BA	1237	A	N1-C6-N6	-18.79	107.33	118.60
26	BA	1755	A	N1-C2-N3	-18.79	119.91	129.30
26	BA	2288	A	C2-N3-C4	18.79	120.00	110.60
26	BA	2639	A	C2-N3-C4	18.79	120.00	110.60
1	AA	143	A	C2-N3-C4	18.79	120.00	110.60
1	AA	161	A	C2-N3-C4	18.79	120.00	110.60
1	AA	327	A	N1-C6-N6	-18.79	107.33	118.60
1	AA	716	A	C2-N3-C4	18.79	120.00	110.60
1	AA	964	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	1014	A	C2-N3-C4	18.79	119.99	110.60
26	BA	443	A	C2-N3-C4	18.79	120.00	110.60
26	BA	541	A	C2-N3-C4	18.79	120.00	110.60
26	BA	590	A	C2-N3-C4	18.79	120.00	110.60
26	BA	1393	A	C2-N3-C4	18.79	120.00	110.60
26	BA	1504	A	C2-N3-C4	18.79	120.00	110.60
26	BA	1641	A	C2-N3-C4	18.79	120.00	110.60
26	BA	2171	A	C2-N3-C4	18.79	120.00	110.60
26	BA	2369	A	C2-N3-C4	18.79	120.00	110.60
26	BA	2829	A	N1-C6-N6	-18.79	107.33	118.60
1	AA	579	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	665	A	N1-C2-N3	-18.79	119.91	129.30
26	BA	430	A	C2-N3-C4	18.79	119.99	110.60
26	BA	751	A	C2-N3-C4	18.79	119.99	110.60
26	BA	1413	A	N1-C2-N3	-18.79	119.91	129.30
26	BA	1655	A	N1-C2-N3	-18.79	119.91	129.30
26	BA	2614	A	C2-N3-C4	18.79	119.99	110.60
26	BA	2682	A	C2-N3-C4	18.79	119.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	59	A	C2-N3-C4	18.79	119.99	110.60
1	AA	306	A	C2-N3-C4	18.79	119.99	110.60
1	AA	676	A	C2-N3-C4	18.79	119.99	110.60
1	AA	845	A	C2-N3-C4	18.79	119.99	110.60
1	AA	1067	A	C2-N3-C4	18.79	119.99	110.60
25	AY	35	A	C2-N3-C4	18.79	119.99	110.60
26	BA	204	A	C2-N3-C4	18.79	119.99	110.60
26	BA	1070	A	C2-N3-C4	18.79	119.99	110.60
26	BA	1246	A	N1-C6-N6	-18.79	107.33	118.60
26	BA	1515	A	N1-C2-N3	-18.79	119.91	129.30
26	BA	1679	A	C2-N3-C4	18.79	119.99	110.60
26	BA	1690	A	C2-N3-C4	18.79	119.99	110.60
26	BA	2266	A	N1-C6-N6	-18.79	107.33	118.60
1	AA	892	A	C2-N3-C4	18.79	119.99	110.60
1	AA	1288	A	C2-N3-C4	18.79	119.99	110.60
1	AA	1375	A	C2-N3-C4	18.79	119.99	110.60
26	BA	788	A	N1-C2-N3	-18.79	119.91	129.30
26	BA	1515	A	N1-C6-N6	-18.79	107.33	118.60
26	BA	2030	A	N1-C2-N3	-18.79	119.91	129.30
26	BA	2566	A	C2-N3-C4	18.79	119.99	110.60
26	BA	2602	A	C2-N3-C4	18.79	119.99	110.60
26	BA	2823	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	935	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1012	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1022	A	C2-N3-C4	18.78	119.99	110.60
23	AW	38	A	C2-N3-C4	18.78	119.99	110.60
26	BA	160	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	1749	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	1877	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1927	A	C2-N3-C4	18.78	119.99	110.60
27	BB	104	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	554	A	C2-N3-C4	18.78	119.99	110.60
1	AA	759	A	C2-N3-C4	18.78	119.99	110.60
26	BA	507	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	972	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1244	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1701	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	2632	A	C2-N3-C4	18.78	119.99	110.60
26	BA	2781	A	C2-N3-C4	18.78	119.99	110.60
1	AA	155	A	C2-N3-C4	18.78	119.99	110.60
1	AA	243	A	C2-N3-C4	18.78	119.99	110.60
1	AA	509	A	C2-N3-C4	18.78	119.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	648	A	N1-C6-N6	-18.78	107.33	118.60
1	AA	747	A	C2-N3-C4	18.78	119.99	110.60
26	BA	320	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	609	A	C2-N3-C4	18.78	119.99	110.60
26	BA	764	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	1509	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1553	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1591	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1762	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1966	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	2675	A	C2-N3-C4	18.78	119.99	110.60
26	BA	2776	A	C2-N3-C4	18.78	119.99	110.60
26	BA	2886	A	C2-N3-C4	18.78	119.99	110.60
27	BB	50	A	C2-N3-C4	18.78	119.99	110.60
1	AA	583	A	N1-C2-N3	-18.78	119.91	129.30
24	AX	76	A	C2-N3-C4	18.78	119.99	110.60
26	BA	217	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	563	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1086	A	N1-C6-N6	-18.78	107.33	118.60
26	BA	1286	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	1552	A	C2-N3-C4	18.78	119.99	110.60
1	AA	353	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	687	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	996	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1151	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1229	A	N1-C6-N6	-18.78	107.33	118.60
1	AA	1428	A	N1-C6-N6	-18.78	107.33	118.60
1	AA	1434	A	C2-N3-C4	18.78	119.99	110.60
26	BA	216	A	C2-N3-C4	18.78	119.99	110.60
26	BA	344	A	C2-N3-C4	18.78	119.99	110.60
26	BA	705	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1151	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1194	A	N1-C6-N6	-18.78	107.33	118.60
26	BA	1321	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1508	A	C2-N3-C4	18.78	119.99	110.60
26	BA	2031	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	2094	A	C2-N3-C4	18.78	119.99	110.60
1	AA	172	A	N1-C2-N3	-18.78	119.91	129.30
26	BA	101	A	C2-N3-C4	18.78	119.99	110.60
26	BA	241	A	C2-N3-C4	18.78	119.99	110.60
26	BA	505	A	C2-N3-C4	18.78	119.99	110.60
26	BA	1549	A	C2-N3-C4	18.78	119.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	495	A	N1-C2-N3	-18.77	119.91	129.30
1	AA	695	A	C2-N3-C4	18.77	119.99	110.60
1	AA	767	A	C2-N3-C4	18.77	119.99	110.60
1	AA	909	A	N1-C6-N6	-18.77	107.34	118.60
1	AA	1082	A	N1-C2-N3	-18.77	119.91	129.30
1	AA	1111	A	C2-N3-C4	18.77	119.99	110.60
1	AA	1157	A	C2-N3-C4	18.77	119.99	110.60
1	AA	1431	A	C2-N3-C4	18.77	119.99	110.60
24	AX	21	A	C2-N3-C4	18.77	119.99	110.60
26	BA	172	A	C2-N3-C4	18.77	119.99	110.60
26	BA	526	A	N1-C2-N3	-18.77	119.91	129.30
26	BA	637	A	N1-C2-N3	-18.77	119.91	129.30
26	BA	756	A	C2-N3-C4	18.77	119.99	110.60
26	BA	1020	A	C2-N3-C4	18.77	119.99	110.60
26	BA	1327	A	C2-N3-C4	18.77	119.99	110.60
26	BA	1932	A	N1-C2-N3	-18.77	119.91	129.30
26	BA	2281	A	N1-C2-N3	-18.77	119.91	129.30
26	BA	2657	A	N1-C2-N3	-18.77	119.91	129.30
1	AA	10	A	C2-N3-C4	18.77	119.99	110.60
1	AA	1163	A	C2-N3-C4	18.77	119.99	110.60
26	BA	255	A	C2-N3-C4	18.77	119.99	110.60
26	BA	627	A	N1-C2-N3	-18.77	119.91	129.30
26	BA	676	A	C2-N3-C4	18.77	119.99	110.60
1	AA	279	A	C2-N3-C4	18.77	119.99	110.60
1	AA	493	A	C2-N3-C4	18.77	119.99	110.60
1	AA	533	A	N1-C2-N3	-18.77	119.91	129.30
1	AA	983	A	N1-C6-N6	-18.77	107.34	118.60
1	AA	1110	A	C2-N3-C4	18.77	119.99	110.60
23	AW	51	A	C2-N3-C4	18.77	119.99	110.60
26	BA	13	A	C2-N3-C4	18.77	119.98	110.60
26	BA	104	A	C2-N3-C4	18.77	119.99	110.60
26	BA	432	A	C2-N3-C4	18.77	119.98	110.60
26	BA	478	A	N1-C2-N3	-18.77	119.91	129.30
26	BA	613	A	C2-N3-C4	18.77	119.99	110.60
26	BA	1359	A	C2-N3-C4	18.77	119.99	110.60
26	BA	1652	A	N1-C2-N3	-18.77	119.91	129.30
26	BA	2003	A	C2-N3-C4	18.77	119.99	110.60
26	BA	2013	A	C2-N3-C4	18.77	119.99	110.60
26	BA	2154	A	C2-N3-C4	18.77	119.98	110.60
26	BA	2639	A	N1-C2-N3	-18.77	119.92	129.30
26	BA	2748	A	C2-N3-C4	18.77	119.98	110.60
1	AA	246	A	C2-N3-C4	18.77	119.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	532	A	C2-N3-C4	18.77	119.98	110.60
1	AA	1055	A	C2-N3-C4	18.77	119.98	110.60
1	AA	595	A	C2-N3-C4	18.77	119.98	110.60
1	AA	1357	A	C2-N3-C4	18.77	119.98	110.60
26	BA	742	A	N1-C2-N3	-18.77	119.92	129.30
26	BA	918	A	N1-C2-N3	-18.77	119.92	129.30
26	BA	1086	A	N1-C2-N3	-18.77	119.92	129.30
26	BA	1359	A	N1-C2-N3	-18.77	119.92	129.30
26	BA	1637	A	C2-N3-C4	18.77	119.98	110.60
26	BA	1919	A	N1-C6-N6	-18.77	107.34	118.60
26	BA	2142	A	C2-N3-C4	18.77	119.98	110.60
26	BA	2734	A	N1-C6-N6	-18.77	107.34	118.60
1	AA	356	A	C2-N3-C4	18.77	119.98	110.60
1	AA	1046	A	C2-N3-C4	18.77	119.98	110.60
22	AV	15	A	C2-N3-C4	18.77	119.98	110.60
26	BA	1027	A	C2-N3-C4	18.77	119.98	110.60
26	BA	1987	A	N1-C6-N6	-18.77	107.34	118.60
26	BA	2058	A	N1-C2-N3	-18.77	119.92	129.30
26	BA	2740	A	N1-C2-N3	-18.77	119.92	129.30
1	AA	309	A	N1-C2-N3	-18.77	119.92	129.30
1	AA	547	A	C2-N3-C4	18.77	119.98	110.60
1	AA	608	A	C2-N3-C4	18.77	119.98	110.60
1	AA	1191	A	C2-N3-C4	18.77	119.98	110.60
26	BA	126	A	C2-N3-C4	18.77	119.98	110.60
26	BA	167	A	N1-C2-N3	-18.77	119.92	129.30
26	BA	227	A	C2-N3-C4	18.77	119.98	110.60
26	BA	693	A	N1-C6-N6	-18.77	107.34	118.60
26	BA	947	A	C2-N3-C4	18.77	119.98	110.60
26	BA	1156	A	C2-N3-C4	18.77	119.98	110.60
26	BA	1175	A	C2-N3-C4	18.77	119.98	110.60
26	BA	1551	A	C2-N3-C4	18.77	119.98	110.60
27	BB	15	A	N1-C6-N6	-18.77	107.34	118.60
1	AA	10	A	N1-C6-N6	-18.76	107.34	118.60
1	AA	172	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1000	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	1036	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1289	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1299	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	1519	A	C2-N3-C4	18.76	119.98	110.60
24	AX	9	A	C2-N3-C4	18.76	119.98	110.60
26	BA	368	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	911	A	C2-N3-C4	18.76	119.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1254	A	N1-C6-N6	-18.76	107.34	118.60
26	BA	1269	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1977	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1987	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2565	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	349	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	649	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1150	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	1362	A	C2-N3-C4	18.76	119.98	110.60
26	BA	272	A	C2-N3-C4	18.76	119.98	110.60
26	BA	928	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1103	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1505	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1528	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1590	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	1640	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2020	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	2247	A	N1-C6-N6	-18.76	107.34	118.60
26	BA	2899	A	N1-C6-N6	-18.76	107.34	118.60
1	AA	753	A	C2-N3-C4	18.76	119.98	110.60
1	AA	860	A	C2-N3-C4	18.76	119.98	110.60
26	BA	603	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1085	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1302	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	1545	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2020	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2147	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2173	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	2176	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2274	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	2309	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2600	A	N1-C6-N6	-18.76	107.34	118.60
1	AA	28	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1396	A	C2-N3-C4	18.76	119.98	110.60
26	BA	244	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	1522	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2058	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2734	A	C2-N3-C4	18.76	119.98	110.60
1	AA	66	A	C2-N3-C4	18.76	119.98	110.60
1	AA	282	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	288	A	C2-N3-C4	18.76	119.98	110.60
1	AA	451	A	C2-N3-C4	18.76	119.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	878	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	1480	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	556	A	C2-N3-C4	18.76	119.98	110.60
26	BA	575	A	C2-N3-C4	18.76	119.98	110.60
26	BA	643	A	C2-N3-C4	18.76	119.98	110.60
26	BA	821	A	C2-N3-C4	18.76	119.98	110.60
26	BA	959	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	996	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1010	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	1213	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1508	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	2183	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2227	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2706	A	C2-N3-C4	18.76	119.98	110.60
1	AA	274	A	C2-N3-C4	18.76	119.98	110.60
1	AA	718	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	816	A	C2-N3-C4	18.76	119.98	110.60
1	AA	907	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1117	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1441	A	C2-N3-C4	18.76	119.98	110.60
26	BA	217	A	N1-C6-N6	-18.76	107.35	118.60
26	BA	265	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	538	A	N1-C6-N6	-18.76	107.35	118.60
26	BA	616	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	721	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1008	A	C2-N3-C4	18.76	119.98	110.60
26	BA	1254	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	1304	A	N1-C2-N3	-18.76	119.92	129.30
26	BA	1872	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2266	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2273	A	C2-N3-C4	18.76	119.98	110.60
26	BA	2740	A	N1-C6-N6	-18.76	107.35	118.60
1	AA	2	A	C2-N3-C4	18.75	119.98	110.60
1	AA	7	A	C2-N3-C4	18.75	119.98	110.60
1	AA	155	A	N1-C6-N6	-18.75	107.35	118.60
1	AA	171	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	196	A	C2-N3-C4	18.75	119.98	110.60
1	AA	1004	A	C2-N3-C4	18.75	119.98	110.60
23	AW	31	A	C2-N3-C4	18.75	119.98	110.60
26	BA	1284	A	C2-N3-C4	18.75	119.98	110.60
26	BA	1705	A	N1-C2-N3	-18.75	119.92	129.30
26	BA	1969	A	C2-N3-C4	18.75	119.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2090	A	N1-C6-N6	-18.75	107.35	118.60
26	BA	2851	A	C2-N3-C4	18.75	119.98	110.60
1	AA	1274	A	C2-N3-C4	18.75	119.98	110.60
26	BA	925	A	C2-N3-C4	18.75	119.98	110.60
26	BA	1755	A	C2-N3-C4	18.75	119.98	110.60
26	BA	1899	A	C2-N3-C4	18.75	119.98	110.60
26	BA	2322	A	C2-N3-C4	18.75	119.98	110.60
1	AA	80	A	N1-C6-N6	-18.75	107.35	118.60
1	AA	459	A	C2-N3-C4	18.75	119.98	110.60
1	AA	1145	A	C2-N3-C4	18.75	119.98	110.60
1	AA	1238	A	C2-N3-C4	18.75	119.97	110.60
26	BA	677	A	N1-C2-N3	-18.75	119.92	129.30
26	BA	739	A	C2-N3-C4	18.75	119.97	110.60
26	BA	973	A	N1-C6-N6	-18.75	107.35	118.60
26	BA	1129	A	C2-N3-C4	18.75	119.98	110.60
26	BA	1652	A	C2-N3-C4	18.75	119.98	110.60
26	BA	2019	A	N1-C6-N6	-18.75	107.35	118.60
26	BA	2378	A	C2-N3-C4	18.75	119.98	110.60
1	AA	815	A	C2-N3-C4	18.75	119.97	110.60
1	AA	1130	A	C2-N3-C4	18.75	119.97	110.60
1	AA	1213	A	C2-N3-C4	18.75	119.97	110.60
26	BA	1247	A	C2-N3-C4	18.75	119.97	110.60
26	BA	1580	A	C2-N3-C4	18.75	119.97	110.60
26	BA	1801	A	N1-C2-N3	-18.75	119.92	129.30
26	BA	2328	A	C2-N3-C4	18.75	119.97	110.60
1	AA	152	A	C2-N3-C4	18.75	119.97	110.60
1	AA	196	A	N1-C2-N3	-18.75	119.93	129.30
26	BA	668	A	N1-C2-N3	-18.75	119.93	129.30
26	BA	1918	A	C2-N3-C4	18.75	119.97	110.60
26	BA	2015	A	C2-N3-C4	18.75	119.97	110.60
26	BA	2071	A	N1-C6-N6	-18.75	107.35	118.60
26	BA	2169	A	N1-C2-N3	-18.75	119.93	129.30
26	BA	2205	A	C2-N3-C4	18.75	119.97	110.60
26	BA	2635	A	C2-N3-C4	18.75	119.97	110.60
26	BA	2799	A	C2-N3-C4	18.75	119.97	110.60
1	AA	262	A	C2-N3-C4	18.75	119.97	110.60
1	AA	768	A	N1-C2-N3	-18.75	119.93	129.30
26	BA	156	A	N1-C6-N6	-18.75	107.35	118.60
26	BA	575	A	N1-C2-N3	-18.75	119.93	129.30
1	AA	253	A	C2-N3-C4	18.75	119.97	110.60
1	AA	596	A	C2-N3-C4	18.75	119.97	110.60
1	AA	968	A	C2-N3-C4	18.75	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1251	A	N1-C2-N3	-18.75	119.93	129.30
1	AA	1398	A	C2-N3-C4	18.75	119.97	110.60
26	BA	262	A	N1-C2-N3	-18.75	119.93	129.30
26	BA	347	A	N1-C6-N6	-18.75	107.35	118.60
26	BA	603	A	N1-C2-N3	-18.75	119.93	129.30
26	BA	734	A	C2-N3-C4	18.75	119.97	110.60
26	BA	1046	A	N1-C2-N3	-18.75	119.93	129.30
26	BA	1713	A	C2-N3-C4	18.75	119.97	110.60
26	BA	2314	A	N1-C2-N3	-18.75	119.93	129.30
1	AA	702	A	C2-N3-C4	18.74	119.97	110.60
26	BA	1705	A	C2-N3-C4	18.74	119.97	110.60
26	BA	1757	A	C2-N3-C4	18.74	119.97	110.60
26	BA	2274	A	C2-N3-C4	18.74	119.97	110.60
1	AA	205	A	C2-N3-C4	18.74	119.97	110.60
1	AA	383	A	C2-N3-C4	18.74	119.97	110.60
1	AA	456	A	N1-C6-N6	-18.74	107.35	118.60
1	AA	461	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1067	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	1287	A	C2-N3-C4	18.74	119.97	110.60
26	BA	513	A	C2-N3-C4	18.74	119.97	110.60
26	BA	899	A	C2-N3-C4	18.74	119.97	110.60
26	BA	945	A	C2-N3-C4	18.74	119.97	110.60
26	BA	973	A	C2-N3-C4	18.74	119.97	110.60
26	BA	1347	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	1434	A	C2-N3-C4	18.74	119.97	110.60
26	BA	1932	A	N1-C6-N6	-18.74	107.35	118.60
26	BA	2336	A	C2-N3-C4	18.74	119.97	110.60
26	BA	2439	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	2679	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	80	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1238	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	278	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	471	A	C2-N3-C4	18.74	119.97	110.60
26	BA	482	A	C2-N3-C4	18.74	119.97	110.60
26	BA	515	A	C2-N3-C4	18.74	119.97	110.60
26	BA	1039	A	C2-N3-C4	18.74	119.97	110.60
26	BA	1717	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	2434	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1021	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1035	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1229	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1306	A	C2-N3-C4	18.74	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1518	A	C2-N3-C4	18.74	119.97	110.60
26	BA	89	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	156	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	310	A	C2-N3-C4	18.74	119.97	110.60
26	BA	608	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	2135	A	N1-C6-N6	-18.74	107.36	118.60
26	BA	2340	A	C2-N3-C4	18.74	119.97	110.60
26	BA	2358	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	2513	A	C2-N3-C4	18.74	119.97	110.60
1	AA	535	A	C2-N3-C4	18.74	119.97	110.60
26	BA	91	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	270	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	574	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	983	A	N1-C6-N6	-18.74	107.36	118.60
26	BA	1722	A	C2-N3-C4	18.74	119.97	110.60
26	BA	2060	A	C2-N3-C4	18.74	119.97	110.60
26	BA	2534	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	2654	A	C2-N3-C4	18.74	119.97	110.60
26	BA	2887	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	366	A	C2-N3-C4	18.74	119.97	110.60
1	AA	572	A	N1-C6-N6	-18.74	107.36	118.60
1	AA	687	A	C2-N3-C4	18.74	119.97	110.60
1	AA	790	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1155	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1410	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1513	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	716	A	C2-N3-C4	18.74	119.97	110.60
26	BA	927	A	C2-N3-C4	18.74	119.97	110.60
26	BA	1096	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	1586	A	C2-N3-C4	18.74	119.97	110.60
26	BA	1689	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	1780	A	C2-N3-C4	18.74	119.97	110.60
26	BA	2377	A	N1-C2-N3	-18.74	119.93	129.30
26	BA	2670	A	C2-N3-C4	18.74	119.97	110.60
26	BA	2736	A	N1-C2-N3	-18.74	119.93	129.30
27	BB	29	A	N1-C6-N6	-18.74	107.36	118.60
27	BB	66	A	C2-N3-C4	18.74	119.97	110.60
1	AA	190	A	C2-N3-C4	18.73	119.97	110.60
1	AA	559	A	C2-N3-C4	18.73	119.97	110.60
1	AA	704	A	N1-C2-N3	-18.73	119.93	129.30
1	AA	1000	A	C2-N3-C4	18.73	119.97	110.60
1	AA	1246	A	C2-N3-C4	18.73	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1408	A	N1-C2-N3	-18.73	119.93	129.30
1	AA	1413	A	C2-N3-C4	18.73	119.97	110.60
1	AA	1492	A	C2-N3-C4	18.73	119.97	110.60
25	AY	9	A	C2-N3-C4	18.73	119.97	110.60
26	BA	676	A	N1-C2-N3	-18.73	119.93	129.30
26	BA	820	A	C2-N3-C4	18.73	119.97	110.60
26	BA	892	A	C2-N3-C4	18.73	119.97	110.60
26	BA	1189	A	N1-C6-N6	-18.73	107.36	118.60
26	BA	1700	A	C2-N3-C4	18.73	119.97	110.60
26	BA	2497	A	C2-N3-C4	18.73	119.97	110.60
1	AA	139	A	C2-N3-C4	18.73	119.97	110.60
1	AA	238	A	N1-C2-N3	-18.73	119.93	129.30
1	AA	373	A	N1-C2-N3	-18.73	119.93	129.30
26	BA	91	A	C2-N3-C4	18.73	119.97	110.60
26	BA	195	A	C2-N3-C4	18.73	119.97	110.60
26	BA	310	A	N1-C6-N6	-18.73	107.36	118.60
26	BA	311	A	C2-N3-C4	18.73	119.97	110.60
26	BA	432	A	N1-C2-N3	-18.73	119.93	129.30
26	BA	1439	A	C2-N3-C4	18.73	119.97	110.60
26	BA	1502	A	N1-C6-N6	-18.73	107.36	118.60
26	BA	2809	A	N1-C2-N3	-18.73	119.93	129.30
1	AA	72	A	N1-C2-N3	-18.73	119.93	129.30
1	AA	681	A	C2-N3-C4	18.73	119.97	110.60
1	AA	815	A	N1-C2-N3	-18.73	119.93	129.30
1	AA	937	A	C2-N3-C4	18.73	119.97	110.60
1	AA	969	A	C2-N3-C4	18.73	119.97	110.60
26	BA	973	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	979	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	1532	A	C2-N3-C4	18.73	119.97	110.60
26	BA	1885	A	N1-C6-N6	-18.73	107.36	118.60
26	BA	2014	A	C2-N3-C4	18.73	119.97	110.60
26	BA	2212	A	C2-N3-C4	18.73	119.97	110.60
26	BA	2738	A	C2-N3-C4	18.73	119.97	110.60
26	BA	2765	A	N1-C2-N3	-18.73	119.93	129.30
1	AA	282	A	N1-C6-N6	-18.73	107.36	118.60
1	AA	865	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	10	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	84	A	N1-C6-N6	-18.73	107.36	118.60
26	BA	213	A	C2-N3-C4	18.73	119.97	110.60
26	BA	990	A	C2-N3-C4	18.73	119.97	110.60
26	BA	2080	A	C2-N3-C4	18.73	119.97	110.60
26	BA	2482	A	C2-N3-C4	18.73	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	315	A	C2-N3-C4	18.73	119.96	110.60
1	AA	978	A	N1-C6-N6	-18.73	107.36	118.60
23	AW	58	A	C2-N3-C4	18.73	119.97	110.60
26	BA	282	A	C2-N3-C4	18.73	119.96	110.60
26	BA	586	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	676	A	N1-C6-N6	-18.73	107.36	118.60
26	BA	900	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	900	A	N1-C6-N6	-18.73	107.36	118.60
26	BA	941	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	1189	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	1535	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	1803	A	C2-N3-C4	18.73	119.96	110.60
26	BA	2095	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	2191	A	C2-N3-C4	18.73	119.96	110.60
26	BA	2435	A	N1-C2-N3	-18.73	119.94	129.30
1	AA	50	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	412	A	C2-N3-C4	18.73	119.96	110.60
26	BA	844	A	C2-N3-C4	18.73	119.96	110.60
26	BA	1275	A	C2-N3-C4	18.73	119.96	110.60
26	BA	1495	A	C2-N3-C4	18.73	119.96	110.60
26	BA	1597	A	N1-C6-N6	-18.73	107.36	118.60
1	AA	196	A	N1-C6-N6	-18.73	107.36	118.60
23	AW	66	A	C2-N3-C4	18.73	119.96	110.60
26	BA	223	A	N1-C6-N6	-18.73	107.36	118.60
26	BA	614	A	C2-N3-C4	18.73	119.96	110.60
26	BA	1634	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	2270	A	C2-N3-C4	18.73	119.96	110.60
26	BA	2352	A	C2-N3-C4	18.73	119.96	110.60
26	BA	2577	A	C2-N3-C4	18.73	119.96	110.60
26	BA	2639	A	N1-C6-N6	-18.73	107.36	118.60
26	BA	2749	A	N1-C2-N3	-18.73	119.94	129.30
26	BA	2829	A	N1-C2-N3	-18.73	119.94	129.30
1	AA	649	A	N1-C6-N6	-18.72	107.37	118.60
1	AA	900	A	N1-C2-N3	-18.72	119.94	129.30
23	AW	14	A	C2-N3-C4	18.72	119.96	110.60
26	BA	404	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	626	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1147	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1393	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	1509	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	2757	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	807	A	N1-C2-N3	-18.72	119.94	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	923	A	C2-N3-C4	18.72	119.96	110.60
1	AA	974	A	C2-N3-C4	18.72	119.96	110.60
1	AA	1180	A	C2-N3-C4	18.72	119.96	110.60
1	AA	1329	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	1519	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	256	A	C2-N3-C4	18.72	119.96	110.60
26	BA	294	A	C2-N3-C4	18.72	119.96	110.60
26	BA	507	A	C2-N3-C4	18.72	119.96	110.60
26	BA	761	A	C2-N3-C4	18.72	119.96	110.60
26	BA	781	A	C2-N3-C4	18.72	119.96	110.60
26	BA	789	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1347	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1431	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1525	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1572	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1809	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	2031	A	N1-C6-N6	-18.72	107.37	118.60
26	BA	2037	A	C2-N3-C4	18.72	119.96	110.60
26	BA	2590	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	2679	A	C2-N3-C4	18.72	119.96	110.60
26	BA	2882	A	N1-C6-N6	-18.72	107.37	118.60
1	AA	715	A	C2-N3-C4	18.72	119.96	110.60
1	AA	1055	A	N1-C6-N6	-18.72	107.37	118.60
1	AA	1155	A	N1-C6-N6	-18.72	107.37	118.60
26	BA	182	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1420	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1815	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	2030	A	N1-C6-N6	-18.72	107.37	118.60
26	BA	2170	A	C2-N3-C4	18.72	119.96	110.60
26	BA	2662	A	C2-N3-C4	18.72	119.96	110.60
26	BA	2750	A	C2-N3-C4	18.72	119.96	110.60
1	AA	728	A	C2-N3-C4	18.72	119.96	110.60
1	AA	959	A	C2-N3-C4	18.72	119.96	110.60
1	AA	1508	A	C2-N3-C4	18.72	119.96	110.60
26	BA	483	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	538	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1020	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	1111	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1142	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	1477	A	C2-N3-C4	18.72	119.96	110.60
26	BA	1635	A	N1-C6-N6	-18.72	107.37	118.60
26	BA	1735	A	C2-N3-C4	18.72	119.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1819	A	N1-C6-N6	-18.72	107.37	118.60
26	BA	1987	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	2009	A	C2-N3-C4	18.72	119.96	110.60
26	BA	2101	A	N1-C6-N6	-18.72	107.37	118.60
26	BA	2572	A	C2-N3-C4	18.72	119.96	110.60
1	AA	320	A	N1-C6-N6	-18.72	107.37	118.60
1	AA	349	A	N1-C6-N6	-18.72	107.37	118.60
1	AA	441	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	94	A	C2-N3-C4	18.72	119.96	110.60
26	BA	345	A	C2-N3-C4	18.72	119.96	110.60
26	BA	453	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	753	A	C2-N3-C4	18.72	119.96	110.60
1	AA	298	A	C2-N3-C4	18.72	119.96	110.60
1	AA	573	A	N1-C6-N6	-18.72	107.37	118.60
1	AA	996	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	1101	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	502	A	N1-C2-N3	-18.72	119.94	129.30
26	BA	829	A	C2-N3-C4	18.72	119.96	110.60
26	BA	2412	A	C2-N3-C4	18.72	119.96	110.60
26	BA	2448	A	C2-N3-C4	18.72	119.96	110.60
26	BA	2589	A	C2-N3-C4	18.72	119.96	110.60
27	BB	50	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	383	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	814	A	C2-N3-C4	18.71	119.96	110.60
26	BA	38	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	340	A	C2-N3-C4	18.71	119.96	110.60
26	BA	415	A	C2-N3-C4	18.71	119.96	110.60
26	BA	743	A	C2-N3-C4	18.71	119.96	110.60
26	BA	981	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	1744	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	2114	A	N1-C6-N6	-18.71	107.37	118.60
1	AA	66	A	N1-C6-N6	-18.71	107.37	118.60
1	AA	101	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	162	A	C2-N3-C4	18.71	119.96	110.60
1	AA	336	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	802	A	N1-C6-N6	-18.71	107.37	118.60
1	AA	1447	A	C2-N3-C4	18.71	119.96	110.60
1	AA	1531	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	71	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	457	A	C2-N3-C4	18.71	119.96	110.60
26	BA	1129	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	1384	A	N1-C2-N3	-18.71	119.94	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1413	A	N1-C6-N6	-18.71	107.37	118.60
26	BA	1815	A	C2-N3-C4	18.71	119.96	110.60
26	BA	1819	A	C2-N3-C4	18.71	119.96	110.60
27	BB	53	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	8	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	673	A	N1-C2-N3	-18.71	119.94	129.30
22	AV	17	A	C2-N3-C4	18.71	119.96	110.60
25	AY	14	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	1073	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	1739	A	C2-N3-C4	18.71	119.96	110.60
26	BA	2813	A	C2-N3-C4	18.71	119.96	110.60
1	AA	19	A	N1-C6-N6	-18.71	107.37	118.60
1	AA	253	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	468	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	510	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	583	A	N1-C6-N6	-18.71	107.37	118.60
1	AA	1465	A	C2-N3-C4	18.71	119.95	110.60
26	BA	104	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	905	A	C2-N3-C4	18.71	119.95	110.60
26	BA	1677	A	C2-N3-C4	18.71	119.95	110.60
26	BA	1803	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	1854	A	C2-N3-C4	18.71	119.95	110.60
26	BA	2062	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	2119	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	2135	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	2158	A	N1-C2-N3	-18.71	119.94	129.30
26	BA	2872	A	N1-C2-N3	-18.71	119.94	129.30
27	BB	104	A	N1-C6-N6	-18.71	107.37	118.60
1	AA	130	A	N1-C6-N6	-18.71	107.38	118.60
26	BA	49	A	C2-N3-C4	18.71	119.95	110.60
26	BA	526	A	N1-C6-N6	-18.71	107.38	118.60
26	BA	911	A	N1-C6-N6	-18.71	107.38	118.60
26	BA	1503	A	N1-C6-N6	-18.71	107.37	118.60
26	BA	1786	A	N1-C6-N6	-18.71	107.38	118.60
1	AA	32	A	N1-C2-N3	-18.71	119.95	129.30
1	AA	321	A	C2-N3-C4	18.71	119.95	110.60
1	AA	329	A	C2-N3-C4	18.71	119.95	110.60
1	AA	415	A	N1-C2-N3	-18.71	119.95	129.30
1	AA	602	A	C2-N3-C4	18.71	119.95	110.60
1	AA	1254	A	N1-C2-N3	-18.71	119.95	129.30
1	AA	1275	A	N1-C6-N6	-18.71	107.38	118.60
1	AA	1413	A	N1-C2-N3	-18.71	119.95	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1437	A	N1-C6-N6	-18.71	107.38	118.60
1	AA	1518	A	N1-C2-N3	-18.71	119.95	129.30
26	BA	300	A	N1-C2-N3	-18.71	119.95	129.30
26	BA	402	A	C2-N3-C4	18.71	119.95	110.60
26	BA	1265	A	N1-C6-N6	-18.71	107.38	118.60
26	BA	1322	A	C2-N3-C4	18.71	119.95	110.60
26	BA	2542	A	C2-N3-C4	18.71	119.95	110.60
1	AA	174	A	C2-N3-C4	18.71	119.95	110.60
26	BA	19	A	C2-N3-C4	18.71	119.95	110.60
26	BA	144	A	N1-C2-N3	-18.71	119.95	129.30
26	BA	1711	A	C2-N3-C4	18.71	119.95	110.60
26	BA	1745	A	C2-N3-C4	18.71	119.95	110.60
26	BA	1913	A	C2-N3-C4	18.71	119.95	110.60
27	BB	108	A	C2-N3-C4	18.71	119.95	110.60
1	AA	246	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	520	A	C2-N3-C4	18.70	119.95	110.60
1	AA	819	A	C2-N3-C4	18.70	119.95	110.60
1	AA	1236	A	C2-N3-C4	18.70	119.95	110.60
1	AA	1534	A	N1-C6-N6	-18.70	107.38	118.60
26	BA	309	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	1089	A	C2-N3-C4	18.70	119.95	110.60
26	BA	1522	A	N1-C6-N6	-18.70	107.38	118.60
26	BA	1654	A	C2-N3-C4	18.70	119.95	110.60
1	AA	101	A	C2-N3-C4	18.70	119.95	110.60
1	AA	149	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	574	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	607	A	C2-N3-C4	18.70	119.95	110.60
1	AA	728	A	N1-C6-N6	-18.70	107.38	118.60
1	AA	759	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	1152	A	C2-N3-C4	18.70	119.95	110.60
1	AA	1269	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	1500	A	C2-N3-C4	18.70	119.95	110.60
23	AW	66	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	324	A	N1-C6-N6	-18.70	107.38	118.60
26	BA	1077	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	1783	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	1808	A	C2-N3-C4	18.70	119.95	110.60
26	BA	1978	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	2406	A	C2-N3-C4	18.70	119.95	110.60
26	BA	2531	A	C2-N3-C4	18.70	119.95	110.60
26	BA	447	A	C2-N3-C4	18.70	119.95	110.60
26	BA	655	A	C2-N3-C4	18.70	119.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1009	A	C2-N3-C4	18.70	119.95	110.60
26	BA	1268	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	1698	A	C2-N3-C4	18.70	119.95	110.60
26	BA	1960	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	2366	A	C2-N3-C4	18.70	119.95	110.60
26	BA	2426	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	2753	A	N1-C6-N6	-18.70	107.38	118.60
27	BB	119	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	60	A	C2-N3-C4	18.70	119.95	110.60
1	AA	374	A	C2-N3-C4	18.70	119.95	110.60
1	AA	430	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	554	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	602	A	N1-C6-N6	-18.70	107.38	118.60
1	AA	865	A	C2-N3-C4	18.70	119.95	110.60
1	AA	1239	A	C2-N3-C4	18.70	119.95	110.60
1	AA	1483	A	C2-N3-C4	18.70	119.95	110.60
23	AW	69	A	N1-C6-N6	-18.70	107.38	118.60
26	BA	167	A	N1-C6-N6	-18.70	107.38	118.60
26	BA	223	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	563	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	761	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	1014	A	C2-N3-C4	18.70	119.95	110.60
26	BA	1165	A	C2-N3-C4	18.70	119.95	110.60
26	BA	1603	A	C2-N3-C4	18.70	119.95	110.60
26	BA	2435	A	N1-C6-N6	-18.70	107.38	118.60
26	BA	2542	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	2800	A	C2-N3-C4	18.70	119.95	110.60
27	BB	45	A	C2-N3-C4	18.70	119.95	110.60
27	BB	109	A	C2-N3-C4	18.70	119.95	110.60
1	AA	787	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	1257	A	N1-C2-N3	-18.70	119.95	129.30
25	AY	38	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	74	A	C2-N3-C4	18.70	119.95	110.60
26	BA	300	A	C2-N3-C4	18.70	119.95	110.60
26	BA	504	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	722	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	920	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	2726	A	N1-C2-N3	-18.70	119.95	129.30
27	BB	52	A	C2-N3-C4	18.70	119.95	110.60
1	AA	139	A	N1-C6-N6	-18.70	107.38	118.60
1	AA	313	A	N1-C6-N6	-18.70	107.38	118.60
1	AA	315	A	N1-C2-N3	-18.70	119.95	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	44	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	975	A	C2-N3-C4	18.70	119.95	110.60
26	BA	1009	A	N1-C6-N6	-18.70	107.38	118.60
26	BA	1246	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	1262	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	1284	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	1342	A	N1-C6-N6	-18.70	107.38	118.60
26	BA	1387	A	C2-N3-C4	18.70	119.95	110.60
26	BA	1583	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	2059	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	2530	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	2726	A	C2-N3-C4	18.70	119.95	110.60
26	BA	2860	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	978	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	1111	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	207	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	332	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	538	A	N1-C2-N3	-18.70	119.95	129.30
26	BA	1689	A	N1-C6-N6	-18.70	107.38	118.60
26	BA	1690	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	681	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	749	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	1299	A	N1-C6-N6	-18.69	107.38	118.60
23	AW	73	A	N1-C2-N3	-18.69	119.95	129.30
26	BA	299	A	N1-C6-N6	-18.69	107.38	118.60
26	BA	492	A	C2-N3-C4	18.69	119.95	110.60
26	BA	896	A	N1-C2-N3	-18.69	119.95	129.30
26	BA	1098	A	N1-C2-N3	-18.69	119.95	129.30
26	BA	1301	A	N1-C6-N6	-18.69	107.38	118.60
26	BA	1551	A	N1-C6-N6	-18.69	107.38	118.60
26	BA	1966	A	N1-C6-N6	-18.69	107.38	118.60
26	BA	2097	A	C2-N3-C4	18.69	119.95	110.60
26	BA	2705	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	109	A	C2-N3-C4	18.69	119.95	110.60
1	AA	794	A	C2-N3-C4	18.69	119.95	110.60
1	AA	1201	A	C2-N3-C4	18.69	119.95	110.60
26	BA	466	A	N1-C2-N3	-18.69	119.95	129.30
26	BA	1274	A	N1-C2-N3	-18.69	119.95	129.30
26	BA	1616	A	C2-N3-C4	18.69	119.95	110.60
26	BA	1913	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	223	A	N1-C6-N6	-18.69	107.39	118.60
1	AA	487	A	N1-C2-N3	-18.69	119.95	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	729	A	C2-N3-C4	18.69	119.95	110.60
1	AA	1092	A	C2-N3-C4	18.69	119.94	110.60
26	BA	299	A	N1-C2-N3	-18.69	119.95	129.30
26	BA	1618	A	N1-C2-N3	-18.69	119.95	129.30
26	BA	2183	A	N1-C2-N3	-18.69	119.95	129.30
26	BA	2453	A	N1-C2-N3	-18.69	119.95	129.30
26	BA	2531	A	N1-C2-N3	-18.69	119.95	129.30
26	BA	2547	A	C2-N3-C4	18.69	119.94	110.60
26	BA	2850	A	N1-C2-N3	-18.69	119.95	129.30
27	BB	39	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	977	A	N1-C6-N6	-18.69	107.39	118.60
26	BA	160	A	N1-C6-N6	-18.69	107.39	118.60
26	BA	715	A	C2-N3-C4	18.69	119.94	110.60
26	BA	980	A	N1-C6-N6	-18.69	107.39	118.60
26	BA	1237	A	C2-N3-C4	18.69	119.94	110.60
26	BA	1272	A	N1-C2-N3	-18.69	119.96	129.30
26	BA	2860	A	C2-N3-C4	18.69	119.94	110.60
1	AA	338	A	C2-N3-C4	18.69	119.94	110.60
1	AA	747	A	N1-C2-N3	-18.69	119.96	129.30
1	AA	1196	A	N1-C2-N3	-18.69	119.96	129.30
26	BA	149	A	N1-C2-N3	-18.69	119.96	129.30
26	BA	311	A	N1-C2-N3	-18.69	119.96	129.30
26	BA	1678	A	N1-C2-N3	-18.69	119.96	129.30
26	BA	2810	A	N1-C2-N3	-18.69	119.96	129.30
27	BB	73	A	N1-C6-N6	-18.69	107.39	118.60
1	AA	1082	A	N1-C6-N6	-18.69	107.39	118.60
1	AA	1534	A	N1-C2-N3	-18.69	119.96	129.30
26	BA	1593	A	N1-C2-N3	-18.69	119.96	129.30
1	AA	179	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	792	A	N1-C2-N3	-18.68	119.96	129.30
22	AV	21	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	727	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	829	A	N1-C6-N6	-18.68	107.39	118.60
26	BA	1080	A	C2-N3-C4	18.68	119.94	110.60
26	BA	1085	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	1551	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	1981	A	C2-N3-C4	18.68	119.94	110.60
1	AA	7	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	44	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	300	A	C2-N3-C4	18.68	119.94	110.60
1	AA	493	A	N1-C6-N6	-18.68	107.39	118.60
26	BA	203	A	N1-C6-N6	-18.68	107.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1205	A	C2-N3-C4	18.68	119.94	110.60
26	BA	1268	A	N1-C6-N6	-18.68	107.39	118.60
26	BA	1900	A	C2-N3-C4	18.68	119.94	110.60
26	BA	2198	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	2453	A	N1-C6-N6	-18.68	107.39	118.60
1	AA	465	A	C2-N3-C4	18.68	119.94	110.60
1	AA	547	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	649	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1080	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1428	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1493	A	N1-C6-N6	-18.68	107.39	118.60
26	BA	472	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	764	A	N1-C6-N6	-18.68	107.39	118.60
26	BA	1237	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	1241	A	C2-N3-C4	18.68	119.94	110.60
26	BA	1655	A	C2-N3-C4	18.68	119.94	110.60
26	BA	2082	A	C2-N3-C4	18.68	119.94	110.60
26	BA	2433	A	C2-N3-C4	18.68	119.94	110.60
1	AA	120	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	466	A	C2-N3-C4	18.68	119.94	110.60
1	AA	696	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	974	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	574	A	C2-N3-C4	18.68	119.94	110.60
26	BA	1275	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	1525	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	349	A	C2-N3-C4	18.68	119.94	110.60
1	AA	792	A	N1-C6-N6	-18.68	107.39	118.60
26	BA	21	A	C2-N3-C4	18.68	119.94	110.60
26	BA	497	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	909	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	1383	A	C2-N3-C4	18.68	119.94	110.60
26	BA	1469	A	C2-N3-C4	18.68	119.94	110.60
26	BA	1937	A	C2-N3-C4	18.68	119.94	110.60
26	BA	1998	A	N1-C6-N6	-18.68	107.39	118.60
26	BA	2278	A	C2-N3-C4	18.68	119.94	110.60
26	BA	2333	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	2614	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1081	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1250	A	C2-N3-C4	18.68	119.94	110.60
24	AX	14	A	N1-C6-N6	-18.68	107.39	118.60
26	BA	423	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	2432	A	C2-N3-C4	18.68	119.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2564	A	N1-C6-N6	-18.68	107.39	118.60
1	AA	959	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1288	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1349	A	N1-C6-N6	-18.68	107.39	118.60
26	BA	310	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	677	A	C2-N3-C4	18.68	119.94	110.60
26	BA	1133	A	C2-N3-C4	18.68	119.94	110.60
26	BA	1365	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	1403	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	1544	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	1759	A	C2-N3-C4	18.68	119.94	110.60
26	BA	2268	A	C2-N3-C4	18.68	119.94	110.60
26	BA	2309	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	2425	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	2660	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	2781	A	N1-C2-N3	-18.68	119.96	129.30
26	BA	2814	A	C2-N3-C4	18.68	119.94	110.60
27	BB	101	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	143	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	321	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	1150	A	C2-N3-C4	18.67	119.94	110.60
26	BA	422	A	C2-N3-C4	18.67	119.94	110.60
26	BA	928	A	N1-C2-N3	-18.67	119.96	129.30
26	BA	936	A	N1-C6-N6	-18.67	107.40	118.60
26	BA	983	A	N1-C2-N3	-18.67	119.96	129.30
26	BA	1802	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	456	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	663	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	1246	A	N1-C6-N6	-18.67	107.40	118.60
1	AA	1374	A	C2-N3-C4	18.67	119.94	110.60
1	AA	1468	A	C2-N3-C4	18.67	119.94	110.60
26	BA	632	A	C2-N3-C4	18.67	119.94	110.60
26	BA	819	A	C2-N3-C4	18.67	119.94	110.60
26	BA	878	A	N1-C2-N3	-18.67	119.96	129.30
26	BA	1253	A	C2-N3-C4	18.67	119.94	110.60
26	BA	1433	A	C2-N3-C4	18.67	119.94	110.60
26	BA	1626	A	C2-N3-C4	18.67	119.94	110.60
26	BA	1700	A	N1-C2-N3	-18.67	119.96	129.30
26	BA	2090	A	C2-N3-C4	18.67	119.94	110.60
26	BA	2097	A	N1-C2-N3	-18.67	119.96	129.30
26	BA	2288	A	N1-C6-N6	-18.67	107.40	118.60
26	BA	2734	A	N1-C2-N3	-18.67	119.96	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2809	A	N1-C6-N6	-18.67	107.40	118.60
26	BA	2899	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	228	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	298	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	459	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	482	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	493	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	777	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	1101	A	C2-N3-C4	18.67	119.94	110.60
23	AW	14	A	N1-C2-N3	-18.67	119.96	129.30
26	BA	1496	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	1503	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	1579	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	1616	A	N1-C6-N6	-18.67	107.40	118.60
26	BA	1757	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	1853	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	2600	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	2753	A	C2-N3-C4	18.67	119.94	110.60
1	AA	1271	A	C2-N3-C4	18.67	119.93	110.60
26	BA	28	A	N1-C6-N6	-18.67	107.40	118.60
26	BA	125	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	614	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	189	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	197	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	560	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	975	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	1229	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	1324	A	C2-N3-C4	18.67	119.93	110.60
24	AX	9	A	N1-C6-N6	-18.67	107.40	118.60
25	AY	58	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	111	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	592	A	N1-C6-N6	-18.67	107.40	118.60
26	BA	984	A	C2-N3-C4	18.67	119.93	110.60
26	BA	1143	A	C2-N3-C4	18.67	119.93	110.60
26	BA	1156	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	1677	A	N1-C2-N3	-18.67	119.97	129.30
26	BA	1794	A	N1-C6-N6	-18.67	107.40	118.60
26	BA	2314	A	N1-C6-N6	-18.67	107.40	118.60
26	BA	2654	A	N1-C2-N3	-18.67	119.97	129.30
27	BB	46	A	C2-N3-C4	18.67	119.93	110.60
1	AA	878	A	N1-C6-N6	-18.67	107.40	118.60
26	BA	764	A	C2-N3-C4	18.67	119.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1676	A	C2-N3-C4	18.67	119.93	110.60
26	BA	1821	A	N1-C6-N6	-18.67	107.40	118.60
1	AA	72	A	N1-C6-N6	-18.66	107.40	118.60
1	AA	1188	A	C2-N3-C4	18.66	119.93	110.60
1	AA	1287	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1360	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	340	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	752	A	C2-N3-C4	18.66	119.93	110.60
26	BA	1134	A	C2-N3-C4	18.66	119.93	110.60
26	BA	1155	A	C2-N3-C4	18.66	119.93	110.60
26	BA	1590	A	C2-N3-C4	18.66	119.93	110.60
26	BA	2247	A	C2-N3-C4	18.66	119.93	110.60
1	AA	969	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1163	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1256	A	C2-N3-C4	18.66	119.93	110.60
26	BA	945	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	2101	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	197	A	C2-N3-C4	18.66	119.93	110.60
1	AA	573	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	630	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1145	A	N1-C6-N6	-18.66	107.40	118.60
26	BA	547	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	643	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	877	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	1039	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	1889	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	2051	A	C2-N3-C4	18.66	119.93	110.60
26	BA	2060	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	2721	A	C2-N3-C4	18.66	119.93	110.60
1	AA	50	A	C2-N3-C4	18.66	119.93	110.60
1	AA	946	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	505	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	670	A	C2-N3-C4	18.66	119.93	110.60
26	BA	735	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	980	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	1854	A	N1-C6-N6	-18.66	107.40	118.60
26	BA	2358	A	C2-N3-C4	18.66	119.93	110.60
26	BA	2468	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	3	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	246	A	N1-C6-N6	-18.66	107.41	118.60
1	AA	609	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	759	A	N1-C6-N6	-18.66	107.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	878	A	C2-N3-C4	18.66	119.93	110.60
1	AA	969	A	N1-C6-N6	-18.66	107.41	118.60
1	AA	1285	A	C2-N3-C4	18.66	119.93	110.60
22	AV	22	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	219	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	996	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	1420	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	1569	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	1614	A	C2-N3-C4	18.66	119.93	110.60
26	BA	2199	A	N1-C6-N6	-18.66	107.41	118.60
1	AA	161	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1019	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1204	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	1126	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	1754	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	2147	A	N1-C6-N6	-18.66	107.41	118.60
26	BA	2288	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	2572	A	N1-C6-N6	-18.66	107.41	118.60
27	BB	34	A	C2-N3-C4	18.66	119.93	110.60
27	BB	45	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	288	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	344	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	602	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	892	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1280	A	C2-N3-C4	18.66	119.93	110.60
26	BA	127	A	C2-N3-C4	18.66	119.93	110.60
26	BA	199	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	739	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	1095	A	C2-N3-C4	18.66	119.93	110.60
26	BA	1470	A	N1-C2-N3	-18.66	119.97	129.30
26	BA	1821	A	C2-N3-C4	18.66	119.93	110.60
26	BA	1952	A	N1-C6-N6	-18.66	107.41	118.60
26	BA	2392	A	C2-N3-C4	18.66	119.93	110.60
1	AA	1016	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	454	A	C2-N3-C4	18.65	119.93	110.60
26	BA	1057	A	N1-C6-N6	-18.65	107.41	118.60
1	AA	238	A	C2-N3-C4	18.65	119.93	110.60
1	AA	635	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	1318	A	C2-N3-C4	18.65	119.93	110.60
26	BA	165	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	734	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	1230	A	N1-C2-N3	-18.65	119.97	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1392	A	N1-C6-N6	-18.65	107.41	118.60
26	BA	1635	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	2003	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	2227	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	2682	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	364	A	C2-N3-C4	18.65	119.93	110.60
1	AA	781	A	C2-N3-C4	18.65	119.93	110.60
1	AA	1197	A	N1-C6-N6	-18.65	107.41	118.60
25	AY	21	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	42	A	C2-N3-C4	18.65	119.92	110.60
26	BA	528	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	602	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	655	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	78	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	195	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	199	A	N1-C6-N6	-18.65	107.41	118.60
1	AA	250	A	C2-N3-C4	18.65	119.92	110.60
1	AA	279	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	414	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	642	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	816	A	N1-C2-N3	-18.65	119.97	129.30
23	AW	38	A	N1-C2-N3	-18.65	119.98	129.30
24	AX	21	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	83	A	N1-C6-N6	-18.65	107.41	118.60
26	BA	219	A	N1-C6-N6	-18.65	107.41	118.60
26	BA	477	A	C2-N3-C4	18.65	119.92	110.60
26	BA	609	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	1260	A	C2-N3-C4	18.65	119.92	110.60
26	BA	1285	A	C2-N3-C4	18.65	119.92	110.60
26	BA	1285	A	N1-C6-N6	-18.65	107.41	118.60
26	BA	1650	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	1791	A	C2-N3-C4	18.65	119.92	110.60
26	BA	1848	A	C2-N3-C4	18.65	119.92	110.60
26	BA	1858	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	1918	A	N1-C6-N6	-18.65	107.41	118.60
26	BA	1936	A	C2-N3-C4	18.65	119.92	110.60
26	BA	2108	A	C2-N3-C4	18.65	119.92	110.60
26	BA	2147	A	N1-C2-N3	-18.65	119.98	129.30
26	BA	2336	A	N1-C2-N3	-18.65	119.97	129.30
26	BA	2598	A	N1-C2-N3	-18.65	119.98	129.30
1	AA	729	A	N1-C2-N3	-18.65	119.98	129.30
26	BA	936	A	N1-C2-N3	-18.65	119.98	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1287	A	N1-C2-N3	-18.65	119.98	129.30
26	BA	1307	A	N1-C2-N3	-18.65	119.98	129.30
26	BA	2766	A	N1-C2-N3	-18.65	119.98	129.30
1	AA	51	A	N1-C2-N3	-18.65	119.98	129.30
1	AA	152	A	N1-C6-N6	-18.65	107.41	118.60
1	AA	1360	A	N1-C6-N6	-18.65	107.41	118.60
23	AW	41	A	N1-C2-N3	-18.65	119.98	129.30
26	BA	233	A	N1-C2-N3	-18.65	119.98	129.30
26	BA	1028	A	N1-C6-N6	-18.65	107.41	118.60
26	BA	1133	A	N1-C2-N3	-18.65	119.98	129.30
26	BA	1354	A	N1-C2-N3	-18.65	119.98	129.30
26	BA	2600	A	C2-N3-C4	18.65	119.92	110.60
26	BA	2835	A	N1-C6-N6	-18.65	107.41	118.60
1	AA	77	A	C2-N3-C4	18.64	119.92	110.60
1	AA	978	A	C2-N3-C4	18.64	119.92	110.60
26	BA	278	A	N1-C6-N6	-18.64	107.41	118.60
26	BA	1805	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1005	A	C2-N3-C4	18.64	119.92	110.60
1	AA	1513	A	N1-C6-N6	-18.64	107.41	118.60
1	AA	1531	A	N1-C6-N6	-18.64	107.41	118.60
26	BA	89	A	N1-C6-N6	-18.64	107.41	118.60
26	BA	95	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	547	A	N1-C6-N6	-18.64	107.41	118.60
26	BA	990	A	N1-C6-N6	-18.64	107.41	118.60
26	BA	1609	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	2317	A	C2-N3-C4	18.64	119.92	110.60
26	BA	2727	A	N1-C6-N6	-18.64	107.41	118.60
1	AA	977	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1288	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	1322	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	2176	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	2882	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	51	A	C2-N3-C4	18.64	119.92	110.60
1	AA	687	A	N1-C6-N6	-18.64	107.42	118.60
1	AA	1117	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1201	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1250	A	N1-C6-N6	-18.64	107.42	118.60
1	AA	1252	A	C2-N3-C4	18.64	119.92	110.60
23	AW	51	A	N1-C6-N6	-18.64	107.42	118.60
25	AY	73	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	197	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	265	A	N1-C6-N6	-18.64	107.42	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	699	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	1077	A	C2-N3-C4	18.64	119.92	110.60
26	BA	1502	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	1535	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	1672	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	1885	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	1938	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	2572	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	2761	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1502	A	C2-N3-C4	18.64	119.92	110.60
26	BA	429	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	477	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	503	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	528	A	C2-N3-C4	18.64	119.92	110.60
26	BA	631	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	804	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	825	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	1353	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	1385	A	C2-N3-C4	18.64	119.92	110.60
26	BA	1630	A	C2-N3-C4	18.64	119.92	110.60
26	BA	1632	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	1853	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	1871	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	1977	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	2015	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	2434	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	2826	A	C2-N3-C4	18.64	119.92	110.60
1	AA	629	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	648	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1055	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1456	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1513	A	C2-N3-C4	18.64	119.92	110.60
26	BA	781	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	899	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	1054	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	1773	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	1780	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	498	A	C2-N3-C4	18.64	119.92	110.60
1	AA	509	A	N1-C6-N6	-18.64	107.42	118.60
1	AA	675	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1285	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1465	A	N1-C2-N3	-18.64	119.98	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	35	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	483	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	508	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	1745	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	2003	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	2513	A	N1-C2-N3	-18.64	119.98	129.30
26	BA	2657	A	N1-C6-N6	-18.64	107.42	118.60
26	BA	2883	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	10	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	914	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	52	A	C2-N3-C4	18.63	119.92	110.60
26	BA	1080	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	1175	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	2369	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	74	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	389	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	435	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	873	A	C2-N3-C4	18.63	119.92	110.60
1	AA	1437	A	C2-N3-C4	18.63	119.92	110.60
1	AA	1480	A	N1-C6-N6	-18.63	107.42	118.60
22	AV	21	A	C2-N3-C4	18.63	119.92	110.60
25	AY	41	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	14	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	666	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	1347	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	2199	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	2266	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	243	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	906	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	1180	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	226	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	508	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	515	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	1285	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	1328	A	N1-C2-N3	-18.63	119.98	129.30
26	BA	2198	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	572	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	655	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	1169	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	1246	A	N1-C2-N3	-18.63	119.99	129.30
1	AA	1349	A	N1-C2-N3	-18.63	119.98	129.30
23	AW	59	A	N1-C2-N3	-18.63	119.98	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	213	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	1913	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	2278	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	2448	A	N1-C2-N3	-18.63	119.99	129.30
26	BA	2476	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	2826	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	918	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	104	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	126	A	N1-C2-N3	-18.63	119.99	129.30
26	BA	782	A	C2-N3-C4	18.63	119.91	110.60
26	BA	1609	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	1981	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	2052	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	109	A	N1-C2-N3	-18.63	119.99	129.30
1	AA	116	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	192	A	N1-C2-N3	-18.63	119.99	129.30
1	AA	1219	A	N1-C2-N3	-18.63	119.99	129.30
24	AX	14	A	N1-C2-N3	-18.63	119.99	129.30
26	BA	196	A	N1-C2-N3	-18.63	119.99	129.30
26	BA	262	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	556	A	N1-C2-N3	-18.63	119.99	129.30
26	BA	829	A	N1-C2-N3	-18.63	119.99	129.30
26	BA	844	A	N1-C2-N3	-18.63	119.99	129.30
26	BA	1366	A	N1-C2-N3	-18.63	119.99	129.30
26	BA	1586	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	1618	A	N1-C6-N6	-18.63	107.42	118.60
26	BA	1641	A	N1-C2-N3	-18.63	119.99	129.30
26	BA	2346	A	N1-C2-N3	-18.63	119.99	129.30
26	BA	2530	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	496	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1012	A	N1-C6-N6	-18.62	107.42	118.60
1	AA	1196	A	N1-C6-N6	-18.62	107.42	118.60
23	AW	31	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	13	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	1583	A	N1-C6-N6	-18.62	107.42	118.60
26	BA	2820	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	129	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	205	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	325	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1239	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1239	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	346	A	N1-C6-N6	-18.62	107.43	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	590	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	1134	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	1626	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	1679	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	2476	A	N1-C2-N3	-18.62	119.99	129.30
27	BB	46	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	199	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1110	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	1254	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	63	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	221	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	609	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	2448	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	2893	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	65	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	80	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	790	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	790	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	1042	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1093	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1105	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1176	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	53	A	C2-N3-C4	18.62	119.91	110.60
26	BA	391	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	792	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	959	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	1327	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	563	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	768	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	191	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	443	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	1001	A	C2-N3-C4	18.62	119.91	110.60
26	BA	1021	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	2270	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	2776	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	2821	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	366	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	451	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	949	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	994	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1413	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	1441	A	N1-C2-N3	-18.62	119.99	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	9	A	N1-C2-N3	-18.62	119.99	129.30
25	AY	6	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	19	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	21	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	251	A	C2-N3-C4	18.62	119.91	110.60
26	BA	422	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	501	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	821	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	1336	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	1395	A	C2-N3-C4	18.62	119.91	110.60
26	BA	2062	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	2614	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	696	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	633	A	C2-N3-C4	18.62	119.91	110.60
26	BA	654	A	N1-C2-N3	-18.62	119.99	129.30
26	BA	742	A	N1-C6-N6	-18.62	107.43	118.60
26	BA	2284	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	59	A	N1-C6-N6	-18.61	107.43	118.60
1	AA	1081	A	N1-C2-N3	-18.61	119.99	129.30
22	AV	20	A	N1-C2-N3	-18.61	119.99	129.30
23	AW	59	A	N1-C6-N6	-18.61	107.43	118.60
26	BA	272	A	N1-C2-N3	-18.61	119.99	129.30
26	BA	439	A	N1-C2-N3	-18.61	119.99	129.30
26	BA	1084	A	N1-C2-N3	-18.61	119.99	129.30
26	BA	1614	A	N1-C2-N3	-18.61	119.99	129.30
26	BA	1918	A	N1-C2-N3	-18.61	119.99	129.30
26	BA	2033	A	C2-N3-C4	18.61	119.91	110.60
26	BA	2503	A	N1-C6-N6	-18.61	107.43	118.60
26	BA	2518	A	N1-C2-N3	-18.61	119.99	129.30
26	BA	2632	A	N1-C2-N3	-18.61	119.99	129.30
26	BA	2733	A	N1-C2-N3	-18.61	119.99	129.30
26	BA	2823	A	N1-C6-N6	-18.61	107.43	118.60
27	BB	66	A	N1-C2-N3	-18.61	119.99	129.30
1	AA	1179	A	N1-C2-N3	-18.61	119.99	129.30
23	AW	21	A	N1-C2-N3	-18.61	119.99	129.30
26	BA	1342	A	N1-C2-N3	-18.61	119.99	129.30
26	BA	2311	A	C2-N3-C4	18.61	119.91	110.60
26	BA	2565	A	N1-C6-N6	-18.61	107.43	118.60
1	AA	3	A	C2-N3-C4	18.61	119.91	110.60
1	AA	780	A	N1-C2-N3	-18.61	119.99	129.30
1	AA	819	A	N1-C2-N3	-18.61	119.99	129.30
1	AA	1499	A	N1-C2-N3	-18.61	119.99	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	320	A	N1-C6-N6	-18.61	107.43	118.60
26	BA	2411	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	2482	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	2587	A	N1-C2-N3	-18.61	119.99	129.30
1	AA	71	A	N1-C6-N6	-18.61	107.43	118.60
1	AA	77	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	181	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	523	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	819	A	N1-C6-N6	-18.61	107.44	118.60
1	AA	1170	A	C2-N3-C4	18.61	119.91	110.60
1	AA	1179	A	N1-C6-N6	-18.61	107.43	118.60
1	AA	1248	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	1319	A	N1-C2-N3	-18.61	120.00	129.30
24	AX	58	A	N1-C6-N6	-18.61	107.44	118.60
26	BA	172	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	1616	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	1872	A	N1-C2-N3	-18.61	120.00	129.30
27	BB	52	A	N1-C6-N6	-18.61	107.44	118.60
27	BB	108	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	1256	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	749	A	C2-N3-C4	18.61	119.90	110.60
26	BA	1746	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	2241	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	393	A	C2-N3-C4	18.61	119.90	110.60
1	AA	465	A	N1-C6-N6	-18.61	107.44	118.60
1	AA	520	A	N1-C6-N6	-18.61	107.44	118.60
1	AA	815	A	N1-C6-N6	-18.61	107.44	118.60
24	AX	58	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	149	A	N1-C6-N6	-18.61	107.44	118.60
26	BA	428	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	844	A	N1-C6-N6	-18.61	107.44	118.60
26	BA	861	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	1155	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	1433	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	1596	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	1596	A	N1-C6-N6	-18.61	107.44	118.60
26	BA	1654	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	1717	A	N1-C6-N6	-18.61	107.44	118.60
26	BA	1786	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	1952	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	2758	A	N1-C2-N3	-18.61	120.00	129.30
27	BB	73	A	N1-C2-N3	-18.61	120.00	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1036	A	N1-C6-N6	-18.61	107.44	118.60
26	BA	911	A	N1-C2-N3	-18.61	120.00	129.30
26	BA	1580	A	N1-C2-N3	-18.61	120.00	129.30
27	BB	94	A	N1-C2-N3	-18.61	120.00	129.30
27	BB	108	A	N1-C6-N6	-18.61	107.44	118.60
1	AA	546	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	621	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	712	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	1042	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	1368	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	1503	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	218	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	478	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	522	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	1548	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	1739	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	2071	A	C2-N3-C4	18.60	119.90	110.60
26	BA	2297	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	71	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	520	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	559	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	825	A	N1-C2-N3	-18.60	120.00	129.30
24	AX	26	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	501	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	1722	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	139	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	574	A	C2-N3-C4	18.60	119.90	110.60
1	AA	676	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	753	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	975	A	C2-N3-C4	18.60	119.90	110.60
26	BA	222	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	391	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	1028	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	1701	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	1847	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	2711	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	2900	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	694	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	702	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	784	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	1503	A	N1-C6-N6	-18.60	107.44	118.60
23	AW	73	A	N1-C6-N6	-18.60	107.44	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	3	A	N1-C2-N3	-18.60	120.00	129.30
25	AY	73	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	221	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	344	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	59	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	502	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	1067	A	N1-C6-N6	-18.60	107.44	118.60
24	AX	26	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	5	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	190	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	374	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	402	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	632	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	654	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	721	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	892	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	917	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	1084	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	1439	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	2358	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	2705	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	448	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	1145	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	1311	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	1492	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	28	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	374	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	878	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	1021	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	1226	A	N1-C2-N3	-18.60	120.00	129.30
26	BA	1230	A	N1-C6-N6	-18.60	107.44	118.60
26	BA	1566	A	C2-N3-C4	18.60	119.90	110.60
26	BA	2883	A	C2-N3-C4	18.60	119.90	110.60
1	AA	78	A	N1-C6-N6	-18.59	107.44	118.60
1	AA	160	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	313	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	1092	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	19	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	83	A	C2-N3-C4	18.59	119.90	110.60
26	BA	213	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	227	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	345	A	N1-C6-N6	-18.59	107.44	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	789	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	1264	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	1365	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	1367	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	1690	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	1809	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	2126	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	2227	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	2602	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	2886	A	N1-C6-N6	-18.59	107.44	118.60
27	BB	101	A	N1-C6-N6	-18.59	107.44	118.60
1	AA	382	A	N1-C6-N6	-18.59	107.44	118.60
1	AA	532	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	1434	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	1447	A	N1-C6-N6	-18.59	107.44	118.60
25	AY	38	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	103	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	1247	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	1366	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	1431	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	2340	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	2850	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	2872	A	N1-C6-N6	-18.59	107.44	118.60
1	AA	152	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	468	A	N1-C6-N6	-18.59	107.44	118.60
1	AA	1271	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	1396	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	10	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	354	A	C2-N3-C4	18.59	119.90	110.60
26	BA	866	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	1431	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	1495	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	1641	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	2042	A	N1-C6-N6	-18.59	107.44	118.60
26	BA	2778	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	441	A	N1-C6-N6	-18.59	107.45	118.60
1	AA	1197	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	1289	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	384	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	429	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	1287	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	1626	A	N1-C6-N6	-18.59	107.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1810	A	C2-N3-C4	18.59	119.89	110.60
26	BA	1889	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	2183	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	2346	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	2376	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	1012	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	1332	A	N1-C6-N6	-18.59	107.45	118.60
22	AV	22	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	348	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	412	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	497	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	793	A	C2-N3-C4	18.59	119.89	110.60
26	BA	1090	A	N1-C2-N3	-18.59	120.00	129.30
26	BA	1586	A	N1-C2-N3	-18.59	120.01	129.30
26	BA	1640	A	N1-C2-N3	-18.59	120.01	129.30
26	BA	1711	A	N1-C2-N3	-18.59	120.01	129.30
26	BA	1744	A	N1-C6-N6	-18.59	107.45	118.60
1	AA	320	A	N1-C2-N3	-18.59	120.01	129.30
1	AA	908	A	C2-N3-C4	18.59	119.89	110.60
26	BA	1787	A	N1-C2-N3	-18.59	120.01	129.30
26	BA	1808	A	N1-C2-N3	-18.59	120.01	129.30
1	AA	913	A	C2-N3-C4	18.59	119.89	110.60
1	AA	1500	A	N1-C6-N6	-18.59	107.45	118.60
1	AA	1519	A	N1-C6-N6	-18.59	107.45	118.60
24	AX	41	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	340	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	590	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	899	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	1050	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	1069	A	N1-C6-N6	-18.59	107.45	118.60
26	BA	1762	A	N1-C2-N3	-18.59	120.01	129.30
26	BA	1927	A	N1-C6-N6	-18.59	107.45	118.60
1	AA	382	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	553	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	1035	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	1492	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	279	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	800	A	C2-N3-C4	18.58	119.89	110.60
26	BA	2482	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	547	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	695	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	780	A	N1-C6-N6	-18.58	107.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	958	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	1046	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	1306	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	1318	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	783	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	920	A	C2-N3-C4	18.58	119.89	110.60
26	BA	927	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	941	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	1046	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	1336	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	1359	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	1927	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	2114	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	2173	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	2738	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	181	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	777	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	816	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	1130	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	1398	A	N1-C2-N3	-18.58	120.01	129.30
25	AY	9	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	146	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	203	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	453	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	727	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	972	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	1698	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	1877	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	2309	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	715	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	718	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	747	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	794	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	913	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	1167	A	N1-C6-N6	-18.58	107.45	118.60
23	AW	76	A	N1-C2-N3	-18.58	120.01	129.30
23	AW	76	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	155	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	988	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	1127	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	1307	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	1571	A	C2-N3-C4	18.58	119.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2873	A	N1-C6-N6	-18.58	107.45	118.60
1	AA	2	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	1340	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	1502	A	N1-C2-N3	-18.58	120.01	129.30
24	AX	76	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	342	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	344	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	943	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	1205	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	1847	A	N1-C6-N6	-18.58	107.45	118.60
27	BB	57	A	N1-C2-N3	-18.58	120.01	129.30
27	BB	94	A	N1-C6-N6	-18.58	107.45	118.60
23	AW	69	A	N1-C2-N3	-18.58	120.01	129.30
25	AY	66	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	362	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	1143	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	1322	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	2851	A	N1-C2-N3	-18.58	120.01	129.30
26	BA	2851	A	N1-C6-N6	-18.58	107.45	118.60
26	BA	2879	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	116	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	167	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	596	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	937	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	974	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	1339	A	N1-C2-N3	-18.57	120.01	129.30
25	AY	23	A	N1-C2-N3	-18.57	120.01	129.30
26	BA	197	A	N1-C6-N6	-18.57	107.45	118.60
26	BA	718	A	N1-C2-N3	-18.57	120.01	129.30
26	BA	1089	A	N1-C2-N3	-18.57	120.01	129.30
26	BA	1089	A	N1-C6-N6	-18.57	107.45	118.60
26	BA	1144	A	N1-C2-N3	-18.57	120.01	129.30
26	BA	2126	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	2268	A	N1-C2-N3	-18.57	120.01	129.30
26	BA	2281	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	2534	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	81	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	872	A	N1-C2-N3	-18.57	120.01	129.30
22	AV	19	A	N1-C2-N3	-18.57	120.01	129.30
23	AW	21	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	63	A	C2-N3-C4	18.57	119.89	110.60
26	BA	71	A	N1-C6-N6	-18.57	107.46	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1095	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	1789	A	C2-N3-C4	18.57	119.89	110.60
1	AA	53	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	119	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	223	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	363	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	364	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	845	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	1431	A	N1-C2-N3	-18.57	120.01	129.30
26	BA	430	A	N1-C2-N3	-18.57	120.02	129.30
26	BA	751	A	N1-C2-N3	-18.57	120.01	129.30
26	BA	788	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	981	A	C2-N3-C4	18.57	119.89	110.60
26	BA	1054	A	N1-C2-N3	-18.57	120.01	129.30
26	BA	1509	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	1900	A	N1-C2-N3	-18.57	120.01	129.30
26	BA	2392	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	2432	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	101	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	448	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	1036	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	1213	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	1375	A	N1-C2-N3	-18.57	120.02	129.30
26	BA	342	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	821	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	1700	A	N1-C6-N6	-18.57	107.46	118.60
27	BB	15	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	197	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	374	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	499	A	C2-N3-C4	18.57	119.88	110.60
1	AA	716	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	946	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	1500	A	N1-C2-N3	-18.57	120.02	129.30
26	BA	309	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	592	A	N1-C2-N3	-18.57	120.02	129.30
26	BA	1050	A	N1-C2-N3	-18.57	120.02	129.30
26	BA	1275	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	1373	A	N1-C2-N3	-18.57	120.02	129.30
26	BA	2378	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	325	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	363	A	N1-C6-N6	-18.57	107.46	118.60
25	AY	41	A	N1-C6-N6	-18.57	107.46	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	66	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	189	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	919	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	1274	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	1377	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	1001	A	N1-C2-N3	-18.57	120.02	129.30
26	BA	1067	A	N1-C2-N3	-18.57	120.02	129.30
26	BA	1264	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	1439	A	N1-C2-N3	-18.57	120.02	129.30
26	BA	1780	A	N1-C6-N6	-18.57	107.46	118.60
26	BA	2758	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	1014	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	1518	A	N1-C6-N6	-18.56	107.46	118.60
26	BA	322	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	945	A	N1-C6-N6	-18.56	107.46	118.60
26	BA	1008	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	1528	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	2748	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	127	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	294	A	N1-C6-N6	-18.56	107.46	118.60
26	BA	507	A	N1-C6-N6	-18.56	107.46	118.60
26	BA	668	A	C2-N3-C4	18.56	119.88	110.60
26	BA	749	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	866	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	1098	A	N1-C6-N6	-18.56	107.46	118.60
26	BA	1490	A	N1-C6-N6	-18.56	107.46	118.60
26	BA	1570	A	C2-N3-C4	18.56	119.88	110.60
26	BA	1821	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	2042	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	2406	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	336	A	C2-N3-C4	18.56	119.88	110.60
1	AA	704	A	N1-C6-N6	-18.56	107.46	118.60
1	AA	1021	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	6	A	N1-C6-N6	-18.56	107.46	118.60
26	BA	73	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	735	A	N1-C6-N6	-18.56	107.46	118.60
1	AA	465	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	906	A	N1-C6-N6	-18.56	107.47	118.60
1	AA	1046	A	N1-C6-N6	-18.56	107.47	118.60
1	AA	1398	A	N1-C6-N6	-18.56	107.46	118.60
1	AA	1433	A	N1-C6-N6	-18.56	107.46	118.60
1	AA	1434	A	N1-C6-N6	-18.56	107.46	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	76	A	N1-C6-N6	-18.56	107.46	118.60
26	BA	294	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	352	A	N1-C6-N6	-18.56	107.46	118.60
26	BA	752	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	1392	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	1434	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	1591	A	N1-C2-N3	-18.56	120.02	129.30
27	BB	115	A	N1-C6-N6	-18.56	107.47	118.60
1	AA	383	A	N1-C6-N6	-18.56	107.47	118.60
26	BA	482	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	492	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	739	A	N1-C6-N6	-18.56	107.47	118.60
26	BA	1008	A	N1-C6-N6	-18.56	107.47	118.60
26	BA	2267	A	N1-C6-N6	-18.56	107.47	118.60
26	BA	2381	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	2411	A	N1-C6-N6	-18.56	107.47	118.60
27	BB	119	A	N1-C6-N6	-18.56	107.47	118.60
1	AA	1251	A	N1-C6-N6	-18.56	107.47	118.60
26	BA	282	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	322	A	C2-N3-C4	18.56	119.88	110.60
26	BA	1383	A	N1-C6-N6	-18.56	107.47	118.60
26	BA	1552	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	1746	A	N1-C6-N6	-18.56	107.47	118.60
26	BA	2108	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	2577	A	N1-C6-N6	-18.56	107.47	118.60
26	BA	2821	A	N1-C6-N6	-18.56	107.47	118.60
26	BA	2886	A	N1-C2-N3	-18.56	120.02	129.30
26	BA	749	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	1039	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	1978	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	2711	A	N1-C2-N3	-18.55	120.02	129.30
1	AA	77	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	1019	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	1346	A	N1-C2-N3	-18.55	120.02	129.30
26	BA	125	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	126	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	2433	A	N1-C2-N3	-18.55	120.02	129.30
1	AA	120	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	226	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	1067	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	1143	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	2459	A	N1-C2-N3	-18.55	120.02	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	466	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	635	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	996	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	1093	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	1287	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	1362	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	1446	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	1447	A	N1-C2-N3	-18.55	120.02	129.30
26	BA	216	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	348	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	706	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	1048	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	1566	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	1759	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	2274	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	2602	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	2813	A	N1-C2-N3	-18.55	120.02	129.30
1	AA	371	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	600	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	1216	A	C2-N3-C4	18.55	119.87	110.60
1	AA	1499	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	311	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	1678	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	2163	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	1016	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	1483	A	N1-C2-N3	-18.55	120.03	129.30
24	AX	21	A	N1-C6-N6	-18.55	107.47	118.60
25	AY	21	A	N1-C6-N6	-18.55	107.47	118.60
25	AY	69	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	118	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	131	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	382	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	404	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	602	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	616	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	1111	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	1495	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	1569	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	2170	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	2598	A	C2-N3-C4	18.55	119.87	110.60
27	BB	29	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	262	A	N1-C2-N3	-18.55	120.03	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	263	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	958	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	1169	A	N1-C6-N6	-18.55	107.47	118.60
22	AV	17	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	94	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	216	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	833	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	1070	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	1151	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	1302	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	1640	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	1890	A	C2-N3-C4	18.55	119.87	110.60
26	BA	2541	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	2577	A	N1-C2-N3	-18.55	120.03	129.30
26	BA	2726	A	N1-C6-N6	-18.55	107.47	118.60
26	BA	2893	A	N1-C6-N6	-18.55	107.47	118.60
27	BB	58	A	C2-N3-C4	18.55	119.87	110.60
27	BB	99	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	74	A	C2-N3-C4	18.54	119.87	110.60
1	AA	149	A	N1-C6-N6	-18.54	107.47	118.60
1	AA	155	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	332	A	N1-C6-N6	-18.54	107.47	118.60
26	BA	637	A	N1-C6-N6	-18.54	107.47	118.60
26	BA	1494	A	N1-C6-N6	-18.54	107.47	118.60
26	BA	2051	A	N1-C6-N6	-18.54	107.47	118.60
1	AA	374	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	706	A	N1-C6-N6	-18.54	107.47	118.60
1	AA	1110	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1188	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	586	A	N1-C6-N6	-18.54	107.47	118.60
26	BA	1088	A	N1-C6-N6	-18.54	107.47	118.60
26	BA	1757	A	N1-C6-N6	-18.54	107.47	118.60
26	BA	2014	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	2058	A	N1-C6-N6	-18.54	107.47	118.60
1	AA	16	A	C2-N3-C4	18.54	119.87	110.60
1	AA	306	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	461	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1004	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1146	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	1572	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	2378	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	2873	A	N1-C2-N3	-18.54	120.03	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	298	A	N1-C6-N6	-18.54	107.48	118.60
1	AA	338	A	N1-C6-N6	-18.54	107.48	118.60
1	AA	466	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1250	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	13	A	N1-C6-N6	-18.54	107.48	118.60
26	BA	892	A	N1-C6-N6	-18.54	107.48	118.60
26	BA	1453	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	1505	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1433	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	947	A	N1-C6-N6	-18.54	107.48	118.60
26	BA	1877	A	N1-C6-N6	-18.54	107.48	118.60
1	AA	607	A	N1-C6-N6	-18.54	107.48	118.60
1	AA	676	A	N1-C6-N6	-18.54	107.48	118.60
1	AA	864	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1171	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1377	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1430	A	N1-C2-N3	-18.54	120.03	129.30
22	AV	17	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	161	A	C2-N3-C4	18.54	119.87	110.60
26	BA	447	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	721	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	1194	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	1247	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	2054	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	2376	A	C2-N3-C4	18.54	119.87	110.60
26	BA	2814	A	N1-C6-N6	-18.54	107.48	118.60
1	AA	250	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	600	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1111	A	N1-C6-N6	-18.54	107.48	118.60
1	AA	1227	A	N1-C6-N6	-18.54	107.48	118.60
23	AW	9	A	N1-C2-N3	-18.54	120.03	129.30
26	BA	1384	A	N1-C6-N6	-18.54	107.48	118.60
26	BA	1420	A	N1-C6-N6	-18.54	107.48	118.60
26	BA	2468	A	N1-C6-N6	-18.54	107.48	118.60
1	AA	174	A	N1-C2-N3	-18.53	120.03	129.30
1	AA	274	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	695	A	N1-C2-N3	-18.53	120.03	129.30
1	AA	807	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	1117	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	144	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	1490	A	N1-C2-N3	-18.53	120.03	129.30
26	BA	1525	A	N1-C6-N6	-18.53	107.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2117	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	2542	A	N1-C6-N6	-18.53	107.48	118.60
27	BB	115	A	N1-C2-N3	-18.53	120.03	129.30
1	AA	300	A	N1-C2-N3	-18.53	120.03	129.30
1	AA	694	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	1257	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	1274	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	504	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	613	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	1175	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	2270	A	N1-C2-N3	-18.53	120.03	129.30
1	AA	50	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	228	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	900	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	1236	A	N1-C2-N3	-18.53	120.03	129.30
22	AV	21	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	218	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	270	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	412	A	N1-C2-N3	-18.53	120.03	129.30
26	BA	1088	A	N1-C2-N3	-18.53	120.03	129.30
26	BA	1321	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	2328	A	N1-C2-N3	-18.53	120.03	129.30
26	BA	2433	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	2750	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	236	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	640	A	N1-C2-N3	-18.53	120.03	129.30
26	BA	103	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	172	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	699	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	1142	A	C2-N3-C4	18.53	119.86	110.60
26	BA	2820	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	8	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	535	A	N1-C6-N6	-18.53	107.48	118.60
23	AW	58	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	14	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	716	A	N1-C2-N3	-18.53	120.04	129.30
26	BA	743	A	N1-C2-N3	-18.53	120.04	129.30
26	BA	1205	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	1580	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	1632	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	1848	A	N1-C2-N3	-18.53	120.04	129.30
26	BA	1890	A	N1-C6-N6	-18.53	107.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2005	A	N1-C2-N3	-18.53	120.04	129.30
1	AA	33	A	N1-C2-N3	-18.53	120.04	129.30
1	AA	663	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	968	A	N1-C2-N3	-18.53	120.04	129.30
1	AA	1332	A	N1-C2-N3	-18.53	120.04	129.30
26	BA	1802	A	N1-C6-N6	-18.53	107.48	118.60
26	BA	2738	A	N1-C6-N6	-18.53	107.48	118.60
1	AA	143	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	274	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	315	A	N1-C6-N6	-18.52	107.48	118.60
1	AA	502	A	C2-N3-C4	18.52	119.86	110.60
1	AA	787	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	1014	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	1092	A	N1-C6-N6	-18.52	107.48	118.60
1	AA	1176	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	73	A	C2-N3-C4	18.52	119.86	110.60
26	BA	74	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	101	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	627	A	N1-C6-N6	-18.52	107.48	118.60
26	BA	896	A	N1-C6-N6	-18.52	107.48	118.60
26	BA	1650	A	N1-C6-N6	-18.52	107.48	118.60
26	BA	1900	A	N1-C6-N6	-18.52	107.48	118.60
26	BA	2426	A	N1-C6-N6	-18.52	107.48	118.60
1	AA	415	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	384	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	655	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	1029	A	C2-N3-C4	18.52	119.86	110.60
26	BA	1669	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	2015	A	N1-C2-N3	-18.52	120.04	129.30
27	BB	39	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	461	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	673	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	831	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	1408	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	1430	A	N1-C6-N6	-18.52	107.49	118.60
24	AX	41	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	477	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	626	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	626	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	666	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	670	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	1301	A	N1-C2-N3	-18.52	120.04	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1597	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	1735	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	1819	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	2211	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	2727	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	83	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	2765	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	574	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	607	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	368	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	563	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	1544	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	2887	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	236	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	181	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	1321	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	1654	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	1676	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	753	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	1170	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	1280	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	1329	A	C2-N3-C4	18.52	119.86	110.60
26	BA	345	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	613	A	N1-C2-N3	-18.52	120.04	129.30
26	BA	988	A	C2-N3-C4	18.52	119.86	110.60
26	BA	1272	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	1808	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	2037	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	2311	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	2679	A	N1-C6-N6	-18.52	107.49	118.60
26	BA	2700	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	595	A	N1-C2-N3	-18.51	120.04	129.30
1	AA	1130	A	N1-C6-N6	-18.51	107.49	118.60
26	BA	1679	A	N1-C6-N6	-18.51	107.49	118.60
26	BA	2518	A	N1-C6-N6	-18.51	107.49	118.60
27	BB	109	A	N1-C2-N3	-18.51	120.04	129.30
1	AA	336	A	N1-C6-N6	-18.51	107.49	118.60
1	AA	1431	A	N1-C6-N6	-18.51	107.49	118.60
23	AW	31	A	N1-C6-N6	-18.51	107.49	118.60
26	BA	432	A	N1-C6-N6	-18.51	107.49	118.60
26	BA	1103	A	N1-C2-N3	-18.51	120.04	129.30
26	BA	2565	A	C2-N3-C4	18.51	119.86	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2733	A	N1-C6-N6	-18.51	107.49	118.60
26	BA	2750	A	N1-C2-N3	-18.51	120.04	129.30
1	AA	51	A	N1-C6-N6	-18.51	107.49	118.60
1	AA	715	A	N1-C6-N6	-18.51	107.49	118.60
1	AA	794	A	N1-C2-N3	-18.51	120.05	129.30
1	AA	1080	A	N1-C6-N6	-18.51	107.49	118.60
1	AA	1429	A	N1-C2-N3	-18.51	120.04	129.30
26	BA	792	A	N1-C6-N6	-18.51	107.49	118.60
26	BA	1032	A	C2-N3-C4	18.51	119.86	110.60
26	BA	1453	A	N1-C6-N6	-18.51	107.49	118.60
26	BA	1549	A	N1-C2-N3	-18.51	120.05	129.30
1	AA	366	A	N1-C2-N3	-18.51	120.05	129.30
1	AA	432	A	N1-C6-N6	-18.51	107.50	118.60
1	AA	1324	A	N1-C2-N3	-18.51	120.05	129.30
26	BA	479	A	C2-N3-C4	18.51	119.85	110.60
26	BA	586	A	C2-N3-C4	18.51	119.86	110.60
26	BA	1854	A	N1-C2-N3	-18.51	120.05	129.30
26	BA	2191	A	N1-C2-N3	-18.51	120.05	129.30
26	BA	2212	A	N1-C6-N6	-18.51	107.49	118.60
1	AA	460	A	N1-C2-N3	-18.51	120.05	129.30
1	AA	559	A	N1-C6-N6	-18.51	107.50	118.60
26	BA	49	A	N1-C2-N3	-18.51	120.05	129.30
26	BA	94	A	N1-C6-N6	-18.51	107.50	118.60
26	BA	118	A	N1-C2-N3	-18.51	120.05	129.30
26	BA	347	A	N1-C2-N3	-18.51	120.05	129.30
26	BA	541	A	N1-C6-N6	-18.51	107.50	118.60
26	BA	716	A	N1-C6-N6	-18.51	107.50	118.60
26	BA	789	A	N1-C6-N6	-18.51	107.50	118.60
26	BA	1373	A	N1-C6-N6	-18.51	107.50	118.60
1	AA	1191	A	N1-C6-N6	-18.51	107.50	118.60
26	BA	863	A	N1-C2-N3	-18.51	120.05	129.30
26	BA	1032	A	N1-C6-N6	-18.51	107.50	118.60
26	BA	1815	A	N1-C6-N6	-18.51	107.50	118.60
1	AA	539	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	655	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	919	A	C2-N3-C4	18.50	119.85	110.60
26	BA	603	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	730	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	1027	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	1111	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	1872	A	N1-C6-N6	-18.50	107.50	118.60
27	BB	53	A	N1-C6-N6	-18.50	107.50	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	300	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	1027	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	1705	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	2352	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	743	A	N1-C2-N3	-18.50	120.05	129.30
25	AY	35	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	443	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	734	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	1129	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	831	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	705	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	1677	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	2700	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	28	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	288	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	845	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	1261	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	1441	A	N1-C6-N6	-18.50	107.50	118.60
22	AV	15	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	793	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	877	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	1981	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	2013	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	2082	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	2327	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	306	A	N1-C6-N6	-18.50	107.50	118.60
24	AX	23	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	423	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	2634	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	238	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	250	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	629	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	937	A	N1-C6-N6	-18.50	107.50	118.60
1	AA	1261	A	N1-C2-N3	-18.50	120.05	129.30
23	AW	51	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	608	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	670	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	1048	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	1504	A	N1-C2-N3	-18.50	120.05	129.30
26	BA	1672	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	2060	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	2781	A	N1-C6-N6	-18.50	107.50	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2792	A	N1-C6-N6	-18.50	107.50	118.60
26	BA	196	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	401	A	N1-C2-N3	-18.49	120.05	129.30
26	BA	804	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	1134	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	2317	A	N1-C2-N3	-18.49	120.05	129.30
1	AA	19	A	N1-C2-N3	-18.49	120.05	129.30
1	AA	968	A	N1-C6-N6	-18.49	107.50	118.60
1	AA	1022	A	N1-C2-N3	-18.49	120.05	129.30
26	BA	482	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	502	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	761	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	984	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	1269	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	1477	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	1928	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	1936	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	1998	A	N1-C2-N3	-18.49	120.05	129.30
26	BA	2134	A	N1-C2-N3	-18.49	120.05	129.30
26	BA	2434	A	N1-C2-N3	-18.49	120.05	129.30
26	BA	2634	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	2670	A	N1-C2-N3	-18.49	120.05	129.30
26	BA	2670	A	N1-C6-N6	-18.49	107.50	118.60
1	AA	746	A	N1-C2-N3	-18.49	120.05	129.30
26	BA	152	A	N1-C2-N3	-18.49	120.05	129.30
26	BA	782	A	N1-C2-N3	-18.49	120.06	129.30
26	BA	984	A	N1-C2-N3	-18.49	120.06	129.30
26	BA	1151	A	N1-C6-N6	-18.49	107.50	118.60
26	BA	1328	A	N1-C6-N6	-18.49	107.50	118.60
27	BB	109	A	N1-C6-N6	-18.49	107.51	118.60
22	AV	20	A	N1-C6-N6	-18.49	107.51	118.60
26	BA	199	A	N1-C6-N6	-18.49	107.51	118.60
26	BA	1142	A	N1-C6-N6	-18.49	107.51	118.60
26	BA	1477	A	N1-C2-N3	-18.49	120.06	129.30
26	BA	1762	A	N1-C6-N6	-18.49	107.51	118.60
26	BA	2497	A	N1-C6-N6	-18.49	107.51	118.60
26	BA	2660	A	N1-C6-N6	-18.49	107.51	118.60
1	AA	892	A	N1-C6-N6	-18.49	107.51	118.60
1	AA	7	A	N1-C6-N6	-18.49	107.51	118.60
1	AA	270	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	784	A	N1-C6-N6	-18.49	107.51	118.60
1	AA	994	A	N1-C6-N6	-18.49	107.51	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	173	A	N1-C6-N6	-18.49	107.51	118.60
26	BA	1020	A	N1-C6-N6	-18.49	107.51	118.60
26	BA	2019	A	N1-C2-N3	-18.49	120.06	129.30
26	BA	2792	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	712	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	256	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	1009	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	1403	A	N1-C6-N6	-18.48	107.51	118.60
26	BA	2327	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	2675	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	2682	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	190	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	1603	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	1890	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	2170	A	N1-C6-N6	-18.48	107.51	118.60
26	BA	2212	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	2541	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	167	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	901	A	C2-N3-C4	18.48	119.84	110.60
1	AA	913	A	N1-C6-N6	-18.48	107.51	118.60
26	BA	1367	A	N1-C6-N6	-18.48	107.51	118.60
26	BA	2171	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	119	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	553	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	1346	A	N1-C6-N6	-18.48	107.51	118.60
25	AY	26	A	N1-C6-N6	-18.48	107.51	118.60
26	BA	1032	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	1133	A	N1-C6-N6	-18.48	107.51	118.60
26	BA	1969	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	279	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	908	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	925	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	975	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	1101	A	N1-C6-N6	-18.48	107.52	118.60
1	AA	1105	A	N1-C6-N6	-18.48	107.52	118.60
1	AA	1271	A	N1-C6-N6	-18.48	107.51	118.60
26	BA	927	A	N1-C2-N3	-18.48	120.06	129.30
26	BA	2019	A	C2-N3-C4	18.48	119.84	110.60
1	AA	160	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	487	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	715	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	2366	A	N1-C2-N3	-18.47	120.06	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2814	A	N1-C2-N3	-18.47	120.06	129.30
26	BA	2826	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	28	A	N1-C2-N3	-18.47	120.06	129.30
1	AA	767	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	975	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	1269	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	1357	A	N1-C2-N3	-18.47	120.06	129.30
24	AX	24	A	N1-C2-N3	-18.47	120.06	129.30
26	BA	643	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	1274	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	2377	A	N1-C6-N6	-18.47	107.52	118.60
27	BB	57	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	496	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	1350	A	N1-C2-N3	-18.47	120.06	129.30
26	BA	127	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	161	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	1354	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	642	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	864	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	1191	A	N1-C2-N3	-18.47	120.06	129.30
25	AY	14	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	101	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	1608	A	N1-C2-N3	-18.47	120.06	129.30
26	BA	1669	A	N1-C2-N3	-18.47	120.06	129.30
26	BA	1848	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	2317	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	2531	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	2813	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	222	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	1095	A	N1-C2-N3	-18.47	120.07	129.30
26	BA	1655	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	2392	A	N1-C2-N3	-18.47	120.07	129.30
27	BB	52	A	N1-C2-N3	-18.47	120.07	129.30
1	AA	161	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	174	A	N1-C6-N6	-18.47	107.52	118.60
1	AA	596	A	N1-C2-N3	-18.47	120.07	129.30
1	AA	949	A	N1-C2-N3	-18.47	120.07	129.30
25	AY	58	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	422	A	N1-C2-N3	-18.47	120.07	129.30
26	BA	1552	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	1759	A	N1-C6-N6	-18.47	107.52	118.60
26	BA	2856	A	N1-C2-N3	-18.47	120.07	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	595	A	N1-C6-N6	-18.46	107.52	118.60
1	AA	1418	A	N1-C2-N3	-18.46	120.07	129.30
26	BA	352	A	N1-C2-N3	-18.46	120.07	129.30
26	BA	2406	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	2412	A	N1-C2-N3	-18.46	120.07	129.30
27	BB	58	A	N1-C2-N3	-18.46	120.07	129.30
26	BA	6	A	N1-C2-N3	-18.46	120.07	129.30
26	BA	195	A	N1-C2-N3	-18.46	120.07	129.30
26	BA	1433	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	2497	A	N1-C2-N3	-18.46	120.07	129.30
1	AA	1163	A	N1-C6-N6	-18.46	107.52	118.60
1	AA	1396	A	N1-C6-N6	-18.46	107.52	118.60
23	AW	14	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	693	A	N1-C2-N3	-18.46	120.07	129.30
26	BA	996	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	1096	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	1637	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	2080	A	N1-C2-N3	-18.46	120.07	129.30
1	AA	263	A	C2-N3-C4	18.46	119.83	110.60
1	AA	907	A	N1-C2-N3	-18.46	120.07	129.30
1	AA	1216	A	N1-C2-N3	-18.46	120.07	129.30
1	AA	1456	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	428	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	515	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	1080	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	1169	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	1508	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	1528	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	1598	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	1698	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	2278	A	N1-C2-N3	-18.46	120.07	129.30
26	BA	2706	A	N1-C6-N6	-18.46	107.52	118.60
1	AA	65	A	N1-C6-N6	-18.46	107.53	118.60
1	AA	364	A	N1-C6-N6	-18.46	107.53	118.60
26	BA	661	A	N1-C6-N6	-18.46	107.53	118.60
26	BA	2211	A	N1-C6-N6	-18.46	107.53	118.60
26	BA	2425	A	N1-C6-N6	-18.46	107.52	118.60
26	BA	2721	A	N1-C6-N6	-18.46	107.53	118.60
1	AA	303	A	N1-C6-N6	-18.46	107.53	118.60
1	AA	353	A	N1-C6-N6	-18.46	107.53	118.60
26	BA	346	A	N1-C2-N3	-18.46	120.07	129.30
26	BA	470	A	N1-C2-N3	-18.46	120.07	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	479	A	N1-C2-N3	-18.46	120.07	129.30
26	BA	631	A	N1-C6-N6	-18.46	107.53	118.60
26	BA	943	A	N1-C6-N6	-18.46	107.53	118.60
26	BA	1871	A	N1-C6-N6	-18.46	107.53	118.60
1	AA	2	A	N1-C6-N6	-18.46	107.53	118.60
1	AA	964	A	N1-C6-N6	-18.46	107.53	118.60
26	BA	1126	A	N1-C6-N6	-18.46	107.53	118.60
1	AA	344	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	675	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	860	A	N1-C2-N3	-18.45	120.07	129.30
1	AA	1155	A	N1-C2-N3	-18.45	120.07	129.30
26	BA	173	A	N1-C2-N3	-18.45	120.07	129.30
26	BA	782	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	1276	A	N1-C2-N3	-18.45	120.07	129.30
26	BA	1553	A	N1-C2-N3	-18.45	120.07	129.30
26	BA	1579	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	1637	A	N1-C2-N3	-18.45	120.07	129.30
26	BA	2119	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	2721	A	N1-C2-N3	-18.45	120.07	129.30
26	BA	2725	A	N1-C2-N3	-18.45	120.07	129.30
26	BA	2810	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	2900	A	N1-C2-N3	-18.45	120.07	129.30
1	AA	3	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	435	A	N1-C2-N3	-18.45	120.07	129.30
1	AA	1146	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	146	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	195	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	1085	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	1127	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	1284	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	2094	A	N1-C2-N3	-18.45	120.07	129.30
26	BA	2163	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	2635	A	N1-C2-N3	-18.45	120.07	129.30
26	BA	1010	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	1327	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	1953	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	2205	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	303	A	N1-C2-N3	-18.45	120.08	129.30
1	AA	532	A	N1-C6-N6	-18.45	107.53	118.60
23	AW	38	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	44	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	661	A	N1-C2-N3	-18.45	120.08	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1213	A	N1-C2-N3	-18.45	120.08	129.30
26	BA	1739	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	1783	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	1829	A	N1-C2-N3	-18.45	120.08	129.30
26	BA	2059	A	N1-C6-N6	-18.45	107.53	118.60
27	BB	46	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	860	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	718	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	820	A	N1-C2-N3	-18.45	120.08	129.30
26	BA	1789	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	373	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	560	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	630	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	781	A	N1-C2-N3	-18.45	120.08	129.30
1	AA	1213	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	1216	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	833	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	2432	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	60	A	N1-C6-N6	-18.45	107.53	118.60
22	AV	19	A	N1-C6-N6	-18.45	107.53	118.60
26	BA	541	A	N1-C2-N3	-18.44	120.08	129.30
26	BA	753	A	N1-C6-N6	-18.44	107.53	118.60
26	BA	1070	A	N1-C6-N6	-18.44	107.53	118.60
26	BA	1866	A	N1-C2-N3	-18.44	120.08	129.30
26	BA	2088	A	N1-C2-N3	-18.44	120.08	129.30
26	BA	1387	A	N1-C2-N3	-18.44	120.08	129.30
1	AA	498	A	N1-C6-N6	-18.44	107.53	118.60
26	BA	95	A	N1-C6-N6	-18.44	107.54	118.60
26	BA	781	A	N1-C6-N6	-18.44	107.54	118.60
26	BA	979	A	N1-C6-N6	-18.44	107.54	118.60
26	BA	1156	A	N1-C6-N6	-18.44	107.54	118.60
1	AA	1188	A	N1-C6-N6	-18.44	107.54	118.60
1	AA	1285	A	N1-C6-N6	-18.44	107.54	118.60
26	BA	382	A	N1-C2-N3	-18.44	120.08	129.30
26	BA	972	A	N1-C6-N6	-18.44	107.54	118.60
26	BA	1928	A	C2-N3-C4	18.44	119.82	110.60
1	AA	1319	A	N1-C6-N6	-18.44	107.54	118.60
26	BA	255	A	N1-C2-N3	-18.44	120.08	129.30
26	BA	466	A	C2-N3-C4	18.44	119.82	110.60
26	BA	981	A	N1-C6-N6	-18.44	107.54	118.60
1	AA	408	A	C2-N3-C4	18.44	119.82	110.60
1	AA	1502	A	N1-C6-N6	-18.44	107.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	459	A	N1-C6-N6	-18.43	107.54	118.60
1	AA	609	A	N1-C6-N6	-18.43	107.54	118.60
26	BA	793	A	N1-C2-N3	-18.43	120.08	129.30
26	BA	2273	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	1252	A	N1-C6-N6	-18.43	107.54	118.60
26	BA	2407	A	N1-C2-N3	-18.43	120.08	129.30
23	AW	58	A	N1-C2-N3	-18.43	120.08	129.30
26	BA	1253	A	N1-C2-N3	-18.43	120.08	129.30
26	BA	1858	A	N1-C6-N6	-18.43	107.54	118.60
26	BA	2799	A	N1-C2-N3	-18.43	120.08	129.30
26	BA	2883	A	N1-C6-N6	-18.43	107.54	118.60
1	AA	938	A	N1-C2-N3	-18.43	120.08	129.30
26	BA	685	A	N1-C2-N3	-18.43	120.08	129.30
26	BA	928	A	N1-C6-N6	-18.43	107.54	118.60
26	BA	1784	A	N1-C6-N6	-18.43	107.54	118.60
26	BA	2837	A	N1-C2-N3	-18.43	120.08	129.30
26	BA	415	A	N1-C2-N3	-18.43	120.08	129.30
26	BA	1773	A	N1-C6-N6	-18.43	107.54	118.60
26	BA	2369	A	N1-C6-N6	-18.43	107.54	118.60
26	BA	272	A	N1-C6-N6	-18.43	107.54	118.60
1	AA	702	A	N1-C6-N6	-18.43	107.54	118.60
1	AA	1152	A	N1-C2-N3	-18.43	120.09	129.30
26	BA	152	A	N1-C6-N6	-18.43	107.55	118.60
26	BA	556	A	N1-C6-N6	-18.43	107.55	118.60
26	BA	794	A	N1-C2-N3	-18.43	120.09	129.30
26	BA	960	A	N1-C2-N3	-18.43	120.09	129.30
26	BA	1434	A	N1-C6-N6	-18.43	107.54	118.60
26	BA	1754	A	N1-C6-N6	-18.43	107.55	118.60
1	AA	478	A	N1-C2-N3	-18.42	120.09	129.30
26	BA	1916	A	N1-C6-N6	-18.42	107.55	118.60
1	AA	1256	A	N1-C6-N6	-18.42	107.55	118.60
26	BA	575	A	N1-C6-N6	-18.42	107.55	118.60
26	BA	1241	A	N1-C2-N3	-18.42	120.09	129.30
26	BA	2054	A	N1-C6-N6	-18.42	107.55	118.60
26	BA	2654	A	N1-C6-N6	-18.42	107.55	118.60
1	AA	729	A	N1-C6-N6	-18.42	107.55	118.60
1	AA	935	A	N1-C2-N3	-18.42	120.09	129.30
26	BA	582	A	N1-C2-N3	-18.42	120.09	129.30
1	AA	873	A	N1-C2-N3	-18.42	120.09	129.30
26	BA	614	A	N1-C6-N6	-18.42	107.55	118.60
26	BA	2860	A	N1-C6-N6	-18.42	107.55	118.60
27	BB	99	A	N1-C6-N6	-18.42	107.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1144	A	N1-C6-N6	-18.42	107.55	118.60
27	BB	58	A	N1-C6-N6	-18.42	107.55	118.60
1	AA	510	A	N1-C6-N6	-18.41	107.55	118.60
1	AA	1468	A	N1-C2-N3	-18.41	120.09	129.30
1	AA	1507	A	N1-C2-N3	-18.41	120.09	129.30
26	BA	64	A	N1-C6-N6	-18.41	107.55	118.60
26	BA	1608	A	N1-C6-N6	-18.41	107.55	118.60
23	AW	66	A	N1-C6-N6	-18.41	107.55	118.60
26	BA	5	A	N1-C2-N3	-18.41	120.09	129.30
26	BA	751	A	N1-C6-N6	-18.41	107.55	118.60
26	BA	2439	A	N1-C6-N6	-18.41	107.55	118.60
1	AA	1004	A	N1-C6-N6	-18.41	107.55	118.60
26	BA	471	A	N1-C2-N3	-18.41	120.09	129.30
26	BA	1791	A	N1-C2-N3	-18.41	120.09	129.30
26	BA	2665	A	N1-C2-N3	-18.41	120.09	129.30
1	AA	814	A	N1-C2-N3	-18.41	120.10	129.30
1	AA	1446	A	N1-C6-N6	-18.41	107.56	118.60
23	AW	26	A	N1-C2-N3	-18.41	120.10	129.30
26	BA	505	A	N1-C6-N6	-18.41	107.56	118.60
26	BA	1610	A	N1-C6-N6	-18.41	107.56	118.60
26	BA	2184	A	N1-C2-N3	-18.41	120.09	129.30
1	AA	1035	A	N1-C6-N6	-18.41	107.56	118.60
26	BA	176	A	N1-C6-N6	-18.41	107.56	118.60
26	BA	528	A	N1-C6-N6	-18.41	107.56	118.60
26	BA	1505	A	N1-C6-N6	-18.41	107.56	118.60
26	BA	1801	A	N1-C6-N6	-18.41	107.56	118.60
26	BA	2205	A	N1-C2-N3	-18.41	120.10	129.30
1	AA	414	A	N1-C6-N6	-18.40	107.56	118.60
26	BA	1269	A	N1-C2-N3	-18.40	120.10	129.30
26	BA	1504	A	N1-C6-N6	-18.40	107.56	118.60
1	AA	162	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	728	A	N1-C2-N3	-18.40	120.10	129.30
24	AX	3	A	N1-C6-N6	-18.40	107.56	118.60
26	BA	176	A	N1-C2-N3	-18.40	120.10	129.30
26	BA	472	A	N1-C6-N6	-18.40	107.56	118.60
26	BA	849	A	N1-C2-N3	-18.40	120.10	129.30
26	BA	2662	A	N1-C2-N3	-18.40	120.10	129.30
26	BA	715	A	N1-C2-N3	-18.40	120.10	129.30
26	BA	1711	A	N1-C6-N6	-18.40	107.56	118.60
26	BA	2376	A	N1-C6-N6	-18.40	107.56	118.60
1	AA	1375	A	N1-C6-N6	-18.40	107.56	118.60
25	AY	6	A	N1-C6-N6	-18.40	107.56	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	49	A	N1-C6-N6	-18.40	107.56	118.60
26	BA	322	A	N1-C6-N6	-18.40	107.56	118.60
26	BA	750	A	N1-C2-N3	-18.40	120.10	129.30
26	BA	1665	A	N1-C6-N6	-18.40	107.56	118.60
26	BA	2706	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	781	A	N1-C6-N6	-18.40	107.56	118.60
1	AA	918	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	1363	A	N1-C2-N3	-18.40	120.10	129.30
26	BA	2287	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	262	A	N1-C6-N6	-18.39	107.56	118.60
26	BA	503	A	N1-C6-N6	-18.39	107.56	118.60
26	BA	2094	A	N1-C6-N6	-18.39	107.56	118.60
26	BA	2598	A	N1-C6-N6	-18.39	107.56	118.60
1	AA	329	A	N1-C2-N3	-18.39	120.10	129.30
26	BA	1029	A	N1-C2-N3	-18.39	120.10	129.30
26	BA	1169	A	N1-C2-N3	-18.39	120.10	129.30
26	BA	1598	A	C2-N3-C4	18.39	119.80	110.60
1	AA	579	A	N1-C6-N6	-18.39	107.56	118.60
25	AY	9	A	N1-C6-N6	-18.39	107.56	118.60
26	BA	1090	A	N1-C6-N6	-18.39	107.57	118.60
26	BA	1253	A	N1-C6-N6	-18.39	107.56	118.60
26	BA	1393	A	N1-C6-N6	-18.39	107.56	118.60
1	AA	81	A	N1-C6-N6	-18.39	107.57	118.60
1	AA	1180	A	N1-C6-N6	-18.39	107.57	118.60
1	AA	1476	A	N1-C2-N3	-18.39	120.11	129.30
26	BA	1713	A	N1-C6-N6	-18.39	107.57	118.60
26	BA	1735	A	N1-C6-N6	-18.39	107.57	118.60
26	BA	675	A	N1-C6-N6	-18.39	107.57	118.60
26	BA	2267	A	N1-C2-N3	-18.39	120.11	129.30
1	AA	1374	A	N1-C2-N3	-18.39	120.11	129.30
26	BA	439	A	N1-C6-N6	-18.39	107.57	118.60
26	BA	2587	A	N1-C6-N6	-18.39	107.57	118.60
26	BA	2749	A	N1-C6-N6	-18.39	107.57	118.60
26	BA	522	A	N1-C6-N6	-18.38	107.57	118.60
26	BA	2461	A	N1-C2-N3	-18.38	120.11	129.30
26	BA	2516	A	N1-C6-N6	-18.38	107.57	118.60
1	AA	431	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	1508	A	N1-C6-N6	-18.38	107.57	118.60
26	BA	466	A	N1-C6-N6	-18.38	107.57	118.60
26	BA	1912	A	N1-C6-N6	-18.38	107.57	118.60
26	BA	1789	A	N1-C2-N3	-18.38	120.11	129.30
26	BA	2635	A	N1-C6-N6	-18.38	107.57	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	743	A	N1-C6-N6	-18.38	107.57	118.60
26	BA	532	A	N1-C6-N6	-18.38	107.57	118.60
26	BA	2879	A	N1-C6-N6	-18.38	107.57	118.60
1	AA	621	A	N1-C6-N6	-18.38	107.57	118.60
26	BA	1548	A	N1-C6-N6	-18.38	107.57	118.60
26	BA	1938	A	N1-C6-N6	-18.38	107.57	118.60
1	AA	716	A	N1-C6-N6	-18.38	107.57	118.60
26	BA	730	A	N1-C6-N6	-18.38	107.57	118.60
26	BA	2142	A	N1-C2-N3	-18.38	120.11	129.30
26	BA	2837	A	N1-C6-N6	-18.38	107.57	118.60
1	AA	563	A	N1-C6-N6	-18.38	107.58	118.60
1	AA	1306	A	N1-C6-N6	-18.38	107.58	118.60
26	BA	227	A	N1-C6-N6	-18.37	107.58	118.60
26	BA	1226	A	N1-C6-N6	-18.37	107.58	118.60
1	AA	1508	A	N1-C2-N3	-18.37	120.11	129.30
26	BA	820	A	N1-C6-N6	-18.37	107.58	118.60
26	BA	402	A	N1-C6-N6	-18.37	107.58	118.60
26	BA	752	A	N1-C6-N6	-18.37	107.58	118.60
24	AX	23	A	N1-C6-N6	-18.37	107.58	118.60
1	AA	907	A	N1-C6-N6	-18.36	107.58	118.60
1	AA	1362	A	N1-C6-N6	-18.36	107.58	118.60
1	AA	321	A	N1-C6-N6	-18.36	107.58	118.60
26	BA	1469	A	N1-C2-N3	-18.36	120.12	129.30
26	BA	91	A	N1-C6-N6	-18.36	107.58	118.60
26	BA	753	A	N1-C2-N3	-18.36	120.12	129.30
1	AA	478	A	N1-C6-N6	-18.36	107.58	118.60
1	AA	1394	A	N1-C6-N6	-18.36	107.58	118.60
26	BA	675	A	N1-C2-N3	-18.36	120.12	129.30
26	BA	1977	A	N1-C6-N6	-18.36	107.58	118.60
26	BA	1953	A	C2-N3-C4	18.36	119.78	110.60
1	AA	451	A	N1-C6-N6	-18.36	107.59	118.60
26	BA	401	A	N1-C6-N6	-18.36	107.59	118.60
26	BA	925	A	N1-C6-N6	-18.36	107.59	118.60
26	BA	1928	A	N1-C2-N3	-18.36	120.12	129.30
26	BA	2340	A	N1-C6-N6	-18.36	107.59	118.60
1	AA	1171	A	N1-C6-N6	-18.36	107.59	118.60
1	AA	109	A	N1-C6-N6	-18.35	107.59	118.60
1	AA	1236	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	21	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	330	A	N1-C2-N3	-18.35	120.12	129.30
26	BA	1073	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	1470	A	N1-C6-N6	-18.35	107.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1810	A	N1-C2-N3	-18.35	120.12	129.30
26	BA	2169	A	N1-C6-N6	-18.35	107.59	118.60
1	AA	16	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	1103	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	1591	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	231	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	1244	A	N1-C2-N3	-18.35	120.12	129.30
26	BA	1899	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	2461	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	2471	A	N1-C2-N3	-18.35	120.12	129.30
27	BB	66	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	73	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	1383	A	N1-C2-N3	-18.35	120.12	129.30
26	BA	1970	A	N1-C2-N3	-18.35	120.12	129.30
25	AY	69	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	1829	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	1496	A	N1-C6-N6	-18.35	107.59	118.60
26	BA	282	A	N1-C6-N6	-18.34	107.59	118.60
1	AA	371	A	N1-C6-N6	-18.34	107.59	118.60
26	BA	161	A	N1-C2-N3	-18.34	120.13	129.30
26	BA	190	A	N1-C6-N6	-18.34	107.59	118.60
1	AA	1157	A	N1-C2-N3	-18.34	120.13	129.30
1	AA	923	A	N1-C2-N3	-18.34	120.13	129.30
26	BA	449	A	N1-C2-N3	-18.34	120.13	129.30
26	BA	2070	A	N1-C2-N3	-18.34	120.13	129.30
26	BA	2333	A	N1-C6-N6	-18.34	107.60	118.60
26	BA	233	A	N1-C6-N6	-18.34	107.60	118.60
26	BA	689	A	N1-C2-N3	-18.34	120.13	129.30
26	BA	988	A	N1-C2-N3	-18.34	120.13	129.30
26	BA	2328	A	N1-C6-N6	-18.34	107.60	118.60
1	AA	482	A	N1-C6-N6	-18.34	107.60	118.60
26	BA	845	A	N1-C6-N6	-18.34	107.60	118.60
1	AA	460	A	N1-C6-N6	-18.34	107.60	118.60
1	AA	872	A	N1-C6-N6	-18.34	107.60	118.60
26	BA	1260	A	N1-C2-N3	-18.34	120.13	129.30
26	BA	2800	A	N1-C2-N3	-18.34	120.13	129.30
26	BA	492	A	N1-C6-N6	-18.33	107.60	118.60
26	BA	2095	A	N1-C6-N6	-18.33	107.60	118.60
1	AA	608	A	N1-C2-N3	-18.33	120.13	129.30
26	BA	2158	A	N1-C6-N6	-18.33	107.60	118.60
26	BA	2352	A	N1-C6-N6	-18.33	107.60	118.60
26	BA	2516	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	938	A	N1-C6-N6	-18.33	107.60	118.60
26	BA	1787	A	N1-C6-N6	-18.33	107.60	118.60
26	BA	2088	A	N1-C6-N6	-18.33	107.60	118.60
1	AA	1476	A	N1-C6-N6	-18.33	107.61	118.60
26	BA	975	A	N1-C6-N6	-18.33	107.61	118.60
1	AA	1081	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	1429	A	N1-C6-N6	-18.32	107.61	118.60
26	BA	2753	A	N1-C2-N3	-18.32	120.14	129.30
26	BA	64	A	N1-C2-N3	-18.32	120.14	129.30
26	BA	572	A	N1-C6-N6	-18.32	107.61	118.60
26	BA	933	A	N1-C2-N3	-18.32	120.14	129.30
26	BA	1936	A	N1-C2-N3	-18.32	120.14	129.30
26	BA	2284	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	205	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	919	A	N1-C2-N3	-18.32	120.14	129.30
1	AA	1201	A	N1-C6-N6	-18.32	107.61	118.60
25	AY	23	A	N1-C6-N6	-18.32	107.61	118.60
26	BA	706	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	1252	A	N1-C2-N3	-18.31	120.14	129.30
26	BA	2097	A	N1-C6-N6	-18.31	107.61	118.60
1	AA	430	A	N1-C6-N6	-18.31	107.61	118.60
26	BA	1722	A	N1-C6-N6	-18.31	107.61	118.60
26	BA	1899	A	N1-C2-N3	-18.31	120.14	129.30
1	AA	814	A	N1-C6-N6	-18.31	107.61	118.60
26	BA	1395	A	N1-C2-N3	-18.31	120.14	129.30
26	BA	722	A	N1-C6-N6	-18.31	107.62	118.60
26	BA	2386	A	N1-C2-N3	-18.31	120.15	129.30
26	BA	582	A	N1-C6-N6	-18.30	107.62	118.60
1	AA	523	A	N1-C6-N6	-18.30	107.62	118.60
26	BA	750	A	N1-C6-N6	-18.30	107.62	118.60
26	BA	2268	A	N1-C6-N6	-18.30	107.62	118.60
26	BA	2311	A	N1-C2-N3	-18.30	120.15	129.30
26	BA	2386	A	N1-C6-N6	-18.30	107.62	118.60
26	BA	632	A	N1-C2-N3	-18.30	120.15	129.30
1	AA	1465	A	N1-C6-N6	-18.29	107.62	118.60
26	BA	251	A	N1-C2-N3	-18.29	120.15	129.30
1	AA	959	A	N1-C6-N6	-18.29	107.62	118.60
1	AA	32	A	N1-C6-N6	-18.29	107.63	118.60
1	AA	509	A	N1-C2-N3	-18.29	120.16	129.30
1	AA	1219	A	N1-C6-N6	-18.29	107.63	118.60
26	BA	513	A	N1-C2-N3	-18.29	120.16	129.30
26	BA	572	A	N1-C2-N3	-18.29	120.16	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	819	A	N1-C2-N3	-18.29	120.16	129.30
1	AA	55	A	N1-C6-N6	-18.29	107.63	118.60
1	AA	263	A	N1-C2-N3	-18.29	120.16	129.30
26	BA	756	A	N1-C2-N3	-18.29	120.16	129.30
1	AA	55	A	N1-C2-N3	-18.29	120.16	129.30
26	BA	131	A	N1-C2-N3	-18.28	120.16	129.30
26	BA	53	A	N1-C2-N3	-18.28	120.16	129.30
26	BA	2335	A	N1-C2-N3	-18.28	120.16	129.30
26	BA	2776	A	N1-C6-N6	-18.28	107.63	118.60
26	BA	2471	A	N1-C6-N6	-18.28	107.63	118.60
1	AA	270	A	N1-C6-N6	-18.27	107.64	118.60
26	BA	1469	A	N1-C6-N6	-18.27	107.64	118.60
26	BA	2013	A	N1-C6-N6	-18.27	107.64	118.60
26	BA	2665	A	N1-C6-N6	-18.27	107.64	118.60
1	AA	33	A	N1-C6-N6	-18.27	107.64	118.60
26	BA	1077	A	N1-C6-N6	-18.27	107.64	118.60
26	BA	2430	A	N1-C2-N3	-18.27	120.16	129.30
26	BA	2547	A	N1-C2-N3	-18.27	120.17	129.30
26	BA	231	A	N1-C2-N3	-18.27	120.17	129.30
1	AA	640	A	N1-C6-N6	-18.27	107.64	118.60
23	AW	23	A	N1-C2-N3	-18.27	120.17	129.30
26	BA	2184	A	N1-C6-N6	-18.27	107.64	118.60
26	BA	917	A	N1-C6-N6	-18.26	107.64	118.60
26	BA	920	A	N1-C6-N6	-18.26	107.64	118.60
26	BA	2051	A	N1-C2-N3	-18.26	120.17	129.30
26	BA	2142	A	N1-C6-N6	-18.26	107.64	118.60
26	BA	2766	A	N1-C6-N6	-18.26	107.64	118.60
1	AA	1021	A	N1-C6-N6	-18.26	107.64	118.60
26	BA	705	A	N1-C6-N6	-18.26	107.64	118.60
26	BA	794	A	N1-C6-N6	-18.26	107.65	118.60
26	BA	1571	A	N1-C2-N3	-18.26	120.17	129.30
26	BA	2336	A	N1-C6-N6	-18.26	107.64	118.60
27	BB	50	A	N1-C6-N6	-18.26	107.65	118.60
1	AA	1280	A	N1-C6-N6	-18.26	107.65	118.60
26	BA	74	A	N1-C6-N6	-18.25	107.65	118.60
26	BA	1664	A	N1-C2-N3	-18.25	120.17	129.30
1	AA	1324	A	N1-C6-N6	-18.25	107.65	118.60
26	BA	2287	A	N1-C6-N6	-18.25	107.65	118.60
26	BA	2412	A	N1-C6-N6	-18.25	107.65	118.60
26	BA	2407	A	N1-C6-N6	-18.25	107.65	118.60
1	AA	192	A	N1-C6-N6	-18.25	107.65	118.60
25	AY	66	A	N1-C6-N6	-18.25	107.65	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1805	A	N1-C6-N6	-18.25	107.65	118.60
26	BA	2778	A	N1-C6-N6	-18.25	107.65	118.60
26	BA	1610	A	C2-N3-C4	18.24	119.72	110.60
26	BA	142	A	N1-C2-N3	-18.24	120.18	129.30
1	AA	1350	A	N1-C6-N6	-18.24	107.66	118.60
26	BA	52	A	N1-C2-N3	-18.24	120.18	129.30
26	BA	1532	A	N1-C2-N3	-18.24	120.18	129.30
26	BA	2560	A	N1-C2-N3	-18.24	120.18	129.30
1	AA	1044	A	N1-C2-N3	-18.24	120.18	129.30
26	BA	447	A	N1-C6-N6	-18.24	107.66	118.60
1	AA	397	A	N1-C2-N3	-18.23	120.18	129.30
23	AW	26	A	N1-C6-N6	-18.23	107.66	118.60
26	BA	2430	A	N1-C6-N6	-18.23	107.66	118.60
1	AA	1318	A	N1-C6-N6	-18.23	107.66	118.60
26	BA	256	A	N1-C6-N6	-18.23	107.66	118.60
24	AX	24	A	N1-C6-N6	-18.23	107.66	118.60
26	BA	644	A	N1-C2-N3	-18.23	120.19	129.30
1	AA	539	A	N1-C2-N3	-18.23	120.19	129.30
26	BA	1387	A	N1-C6-N6	-18.23	107.67	118.60
26	BA	2459	A	N1-C6-N6	-18.23	107.67	118.60
26	BA	191	A	N1-C6-N6	-18.22	107.67	118.60
1	AA	935	A	N1-C6-N6	-18.22	107.67	118.60
26	BA	415	A	N1-C6-N6	-18.22	107.67	118.60
26	BA	1791	A	N1-C6-N6	-18.22	107.67	118.60
26	BA	2082	A	N1-C6-N6	-18.22	107.67	118.60
1	AA	746	A	N1-C6-N6	-18.22	107.67	118.60
26	BA	1676	A	N1-C6-N6	-18.22	107.67	118.60
1	AA	408	A	N1-C2-N3	-18.21	120.19	129.30
26	BA	1276	A	N1-C6-N6	-18.21	107.67	118.60
26	BA	1664	A	N1-C6-N6	-18.21	107.67	118.60
26	BA	2020	A	N1-C6-N6	-18.21	107.67	118.60
1	AA	1102	A	N1-C2-N3	-18.21	120.19	129.30
26	BA	1603	A	N1-C6-N6	-18.21	107.67	118.60
1	AA	356	A	N1-C6-N6	-18.21	107.68	118.60
26	BA	1566	A	N1-C6-N6	-18.21	107.67	118.60
1	AA	1340	A	N1-C6-N6	-18.20	107.68	118.60
26	BA	2297	A	N1-C6-N6	-18.20	107.68	118.60
1	AA	1483	A	N1-C6-N6	-18.20	107.68	118.60
26	BA	449	A	N1-C6-N6	-18.20	107.68	118.60
26	BA	1353	A	N1-C6-N6	-18.20	107.68	118.60
26	BA	1614	A	N1-C6-N6	-18.19	107.68	118.60
26	BA	1598	A	N1-C2-N3	-18.19	120.20	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1969	A	N1-C6-N6	-18.19	107.69	118.60
26	BA	2547	A	N1-C6-N6	-18.19	107.69	118.60
26	BA	2080	A	N1-C6-N6	-18.18	107.69	118.60
1	AA	1005	A	N1-C2-N3	-18.18	120.21	129.30
26	BA	56	A	N1-C2-N3	-18.18	120.21	129.30
26	BA	2366	A	N1-C6-N6	-18.18	107.69	118.60
26	BA	1745	A	N1-C6-N6	-18.18	107.69	118.60
1	AA	1418	A	N1-C6-N6	-18.18	107.69	118.60
26	BA	1572	A	N1-C6-N6	-18.18	107.69	118.60
1	AA	356	A	N1-C2-N3	-18.18	120.21	129.30
26	BA	743	A	N1-C6-N6	-18.18	107.69	118.60
26	BA	479	A	N1-C6-N6	-18.17	107.70	118.60
26	BA	1494	A	N1-C2-N3	-18.17	120.22	129.30
26	BA	2273	A	N1-C6-N6	-18.17	107.70	118.60
26	BA	2856	A	N1-C6-N6	-18.17	107.70	118.60
1	AA	53	A	N1-C6-N6	-18.17	107.70	118.60
26	BA	1866	A	N1-C6-N6	-18.17	107.70	118.60
27	BB	45	A	N1-C6-N6	-18.16	107.70	118.60
1	AA	1357	A	N1-C6-N6	-18.16	107.70	118.60
26	BA	756	A	N1-C6-N6	-18.16	107.70	118.60
26	BA	845	A	N1-C2-N3	-18.15	120.22	129.30
26	BA	1244	A	N1-C6-N6	-18.15	107.71	118.60
26	BA	644	A	N1-C6-N6	-18.15	107.71	118.60
26	BA	182	A	N1-C2-N3	-18.15	120.23	129.30
26	BA	255	A	N1-C6-N6	-18.14	107.71	118.60
26	BA	1634	A	N1-C6-N6	-18.14	107.71	118.60
26	BA	2014	A	N1-C6-N6	-18.14	107.72	118.60
26	BA	470	A	N1-C6-N6	-18.14	107.72	118.60
1	AA	1022	A	N1-C6-N6	-18.13	107.72	118.60
1	AA	98	A	N1-C2-N3	-18.13	120.23	129.30
26	BA	471	A	N1-C6-N6	-18.13	107.72	118.60
1	AA	1339	A	N1-C6-N6	-18.13	107.72	118.60
26	BA	633	A	N1-C2-N3	-18.13	120.24	129.30
26	BA	2799	A	N1-C6-N6	-18.12	107.72	118.60
26	BA	251	A	N1-C6-N6	-18.12	107.73	118.60
26	BA	430	A	N1-C6-N6	-18.12	107.73	118.60
26	BA	1553	A	N1-C6-N6	-18.12	107.73	118.60
1	AA	495	A	N1-C6-N6	-18.11	107.73	118.60
1	AA	1152	A	N1-C6-N6	-18.11	107.73	118.60
26	BA	1610	A	N1-C2-N3	-18.10	120.25	129.30
26	BA	685	A	N1-C6-N6	-18.10	107.74	118.60
1	AA	1374	A	N1-C6-N6	-18.09	107.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	706	A	N1-C2-N3	-18.09	120.26	129.30
1	AA	901	A	N1-C2-N3	-18.08	120.26	129.30
1	AA	923	A	N1-C6-N6	-18.08	107.75	118.60
26	BA	1571	A	N1-C6-N6	-18.08	107.75	118.60
1	AA	300	A	N1-C6-N6	-18.07	107.76	118.60
26	BA	677	A	N1-C6-N6	-18.07	107.76	118.60
26	BA	1570	A	N1-C2-N3	-18.07	120.26	129.30
1	AA	908	A	N1-C6-N6	-18.07	107.76	118.60
26	BA	2171	A	N1-C6-N6	-18.07	107.76	118.60
26	BA	1532	A	N1-C6-N6	-18.06	107.76	118.60
26	BA	1549	A	N1-C6-N6	-18.06	107.77	118.60
26	BA	2725	A	N1-C6-N6	-18.05	107.77	118.60
26	BA	63	A	N1-C6-N6	-18.04	107.78	118.60
26	BA	933	A	N1-C6-N6	-18.04	107.78	118.60
26	BA	2800	A	N1-C6-N6	-18.04	107.78	118.60
26	BA	2748	A	N1-C6-N6	-18.04	107.78	118.60
1	AA	546	A	N1-C6-N6	-18.03	107.78	118.60
1	AA	1507	A	N1-C6-N6	-18.03	107.78	118.60
1	AA	162	A	N1-C6-N6	-18.02	107.78	118.60
23	AW	23	A	N1-C6-N6	-18.02	107.79	118.60
1	AA	1363	A	N1-C6-N6	-18.02	107.79	118.60
1	AA	1102	A	N1-C6-N6	-18.01	107.79	118.60
26	BA	330	A	N1-C6-N6	-18.00	107.80	118.60
26	BA	142	A	N1-C6-N6	-18.00	107.80	118.60
26	BA	1395	A	N1-C6-N6	-17.99	107.81	118.60
1	AA	865	A	N1-C6-N6	-17.99	107.81	118.60
1	AA	608	A	N1-C6-N6	-17.98	107.81	118.60
26	BA	599	A	N1-C6-N6	-17.98	107.81	118.60
26	BA	1241	A	N1-C6-N6	-17.98	107.81	118.60
26	BA	2191	A	N1-C6-N6	-17.97	107.82	118.60
1	AA	190	A	N1-C6-N6	-17.97	107.82	118.60
1	AA	397	A	N1-C6-N6	-17.96	107.82	118.60
1	AA	1044	A	N1-C6-N6	-17.96	107.83	118.60
1	AA	873	A	N1-C6-N6	-17.95	107.83	118.60
26	BA	2335	A	N1-C6-N6	-17.95	107.83	118.60
1	AA	1468	A	N1-C6-N6	-17.94	107.84	118.60
26	BA	689	A	N1-C6-N6	-17.94	107.83	118.60
26	BA	2675	A	N1-C6-N6	-17.94	107.84	118.60
1	AA	1157	A	N1-C6-N6	-17.93	107.84	118.60
26	BA	513	A	N1-C6-N6	-17.92	107.85	118.60
1	AA	329	A	N1-C6-N6	-17.92	107.85	118.60
26	BA	1029	A	N1-C6-N6	-17.91	107.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1213	A	N1-C6-N6	-17.90	107.86	118.60
26	BA	1970	A	N1-C6-N6	-17.89	107.86	118.60
26	BA	1810	A	N1-C6-N6	-17.89	107.87	118.60
27	BB	59	A	N1-C2-N3	-17.87	120.36	129.30
26	BA	2560	A	N1-C6-N6	-17.86	107.88	118.60
26	BA	56	A	N1-C6-N6	-17.84	107.90	118.60
26	BA	2077	A	N1-C2-N3	-17.82	120.39	129.30
26	BA	863	A	N1-C6-N6	-17.79	107.93	118.60
26	BA	52	A	N1-C6-N6	-17.77	107.94	118.60
26	BA	819	A	N1-C6-N6	-17.75	107.95	118.60
26	BA	599	A	N1-C2-N3	-17.71	120.44	129.30
1	AA	502	A	N1-C6-N6	-17.70	107.98	118.60
1	AA	98	A	N1-C6-N6	-17.66	108.00	118.60
26	BA	960	A	N1-C6-N6	-17.58	108.05	118.60
1	AA	901	A	N1-C6-N6	-17.56	108.06	118.60
1	AA	1005	A	N1-C6-N6	-17.51	108.09	118.60
27	BB	59	A	N1-C6-N6	-17.51	108.09	118.60
26	BA	2662	A	N1-C6-N6	-17.50	108.10	118.60
26	BA	1570	A	N1-C6-N6	-17.38	108.17	118.60
26	BA	1260	A	N1-C6-N6	-17.27	108.24	118.60
26	BA	2077	A	N1-C6-N6	-17.26	108.24	118.60
26	BA	633	A	N1-C6-N6	-17.24	108.26	118.60
1	AA	408	A	N1-C6-N6	-17.03	108.38	118.60
24	AX	16	U	C5-C6-N1	-12.71	116.34	122.70
24	AX	20	U	C5-C6-N1	-12.69	116.36	122.70
23	AW	20	U	C5-C6-N1	-12.67	116.36	122.70
24	AX	19	U	C5-C6-N1	-12.64	116.38	122.70
26	BA	479	A	N7-C8-N9	-12.40	107.60	113.80
1	AA	499	A	N7-C8-N9	-12.29	107.66	113.80
1	AA	1329	A	N7-C8-N9	-12.10	107.75	113.80
1	AA	441	A	N7-C8-N9	-12.05	107.78	113.80
26	BA	1385	A	N7-C8-N9	-11.98	107.81	113.80
26	BA	1655	A	N7-C8-N9	-11.96	107.82	113.80
26	BA	800	A	N7-C8-N9	-11.92	107.84	113.80
1	AA	495	A	N7-C8-N9	-11.90	107.85	113.80
1	AA	1151	A	N7-C8-N9	-11.90	107.85	113.80
26	BA	2388	A	N7-C8-N9	-11.89	107.85	113.80
1	AA	1368	A	N7-C8-N9	-11.89	107.85	113.80
26	BA	371	A	N7-C8-N9	-11.89	107.86	113.80
26	BA	1634	A	N7-C8-N9	-11.88	107.86	113.80
26	BA	204	A	N7-C8-N9	-11.87	107.87	113.80
26	BA	457	A	N7-C8-N9	-11.86	107.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2776	A	N7-C8-N9	-11.84	107.88	113.80
1	AA	915	A	N7-C8-N9	-11.84	107.88	113.80
1	AA	8	A	N7-C8-N9	-11.84	107.88	113.80
26	BA	2542	A	N7-C8-N9	-11.83	107.89	113.80
26	BA	454	A	C5-C6-N6	11.82	133.16	123.70
1	AA	246	A	N7-C8-N9	-11.81	107.89	113.80
1	AA	889	A	N7-C8-N9	-11.80	107.90	113.80
23	AW	51	A	N7-C8-N9	-11.80	107.90	113.80
26	BA	1265	A	N7-C8-N9	-11.80	107.90	113.80
26	BA	1913	A	N7-C8-N9	-11.80	107.90	113.80
27	BB	52	A	N7-C8-N9	-11.79	107.90	113.80
1	AA	51	A	N7-C8-N9	-11.78	107.91	113.80
26	BA	74	A	N7-C8-N9	-11.78	107.91	113.80
1	AA	1239	A	N7-C8-N9	-11.77	107.92	113.80
26	BA	1652	A	N7-C8-N9	-11.77	107.92	113.80
26	BA	265	A	N7-C8-N9	-11.76	107.92	113.80
1	AA	131	A	N7-C8-N9	-11.76	107.92	113.80
23	AW	14	A	N7-C8-N9	-11.76	107.92	113.80
26	BA	677	A	N7-C8-N9	-11.76	107.92	113.80
26	BA	2478	A	N7-C8-N9	-11.76	107.92	113.80
27	BB	34	A	N7-C8-N9	-11.76	107.92	113.80
26	BA	1773	A	N7-C8-N9	-11.75	107.92	113.80
1	AA	583	A	N7-C8-N9	-11.75	107.92	113.80
26	BA	84	A	N7-C8-N9	-11.75	107.92	113.80
26	BA	2009	A	N7-C8-N9	-11.75	107.93	113.80
1	AA	694	A	N7-C8-N9	-11.75	107.93	113.80
1	AA	913	A	N7-C8-N9	-11.75	107.93	113.80
26	BA	1427	A	N7-C8-N9	-11.75	107.93	113.80
24	AX	58	A	N7-C8-N9	-11.74	107.93	113.80
1	AA	767	A	N7-C8-N9	-11.74	107.93	113.80
26	BA	574	A	N7-C8-N9	-11.74	107.93	113.80
26	BA	1509	A	N7-C8-N9	-11.74	107.93	113.80
26	BA	2090	A	N7-C8-N9	-11.74	107.93	113.80
26	BA	2322	A	N7-C8-N9	-11.74	107.93	113.80
26	BA	2418	A	N7-C8-N9	-11.74	107.93	113.80
25	AY	38	A	N7-C8-N9	-11.73	107.94	113.80
26	BA	1960	A	N7-C8-N9	-11.73	107.93	113.80
1	AA	60	A	N7-C8-N9	-11.73	107.94	113.80
1	AA	1408	A	N7-C8-N9	-11.73	107.94	113.80
1	AA	1055	A	N7-C8-N9	-11.72	107.94	113.80
26	BA	320	A	N7-C8-N9	-11.72	107.94	113.80
26	BA	332	A	N7-C8-N9	-11.72	107.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1794	A	N7-C8-N9	-11.72	107.94	113.80
26	BA	2101	A	N7-C8-N9	-11.72	107.94	113.80
1	AA	243	A	N7-C8-N9	-11.71	107.94	113.80
1	AA	753	A	N7-C8-N9	-11.71	107.94	113.80
1	AA	602	A	N7-C8-N9	-11.71	107.95	113.80
26	BA	149	A	N7-C8-N9	-11.70	107.95	113.80
26	BA	1147	A	N7-C8-N9	-11.71	107.95	113.80
1	AA	1155	A	N7-C8-N9	-11.70	107.95	113.80
26	BA	119	A	N7-C8-N9	-11.70	107.95	113.80
26	BA	2758	A	N7-C8-N9	-11.70	107.95	113.80
26	BA	1014	A	N7-C8-N9	-11.70	107.95	113.80
26	BA	2589	A	N7-C8-N9	-11.70	107.95	113.80
26	BA	505	A	N7-C8-N9	-11.69	107.95	113.80
1	AA	197	A	N7-C8-N9	-11.69	107.95	113.80
1	AA	949	A	N7-C8-N9	-11.69	107.95	113.80
26	BA	788	A	N7-C8-N9	-11.69	107.95	113.80
26	BA	1772	A	N7-C8-N9	-11.69	107.95	113.80
1	AA	1179	A	N7-C8-N9	-11.69	107.95	113.80
26	BA	1142	A	N7-C8-N9	-11.69	107.96	113.80
26	BA	1630	A	N7-C8-N9	-11.69	107.96	113.80
1	AA	44	A	N7-C8-N9	-11.69	107.96	113.80
1	AA	181	A	N7-C8-N9	-11.69	107.96	113.80
26	BA	603	A	N7-C8-N9	-11.69	107.96	113.80
26	BA	2082	A	N7-C8-N9	-11.69	107.96	113.80
1	AA	120	A	N7-C8-N9	-11.68	107.96	113.80
22	AV	22	A	N7-C8-N9	-11.68	107.96	113.80
26	BA	2572	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	673	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	759	A	N7-C8-N9	-11.68	107.96	113.80
26	BA	910	A	N7-C8-N9	-11.68	107.96	113.80
26	BA	2031	A	N7-C8-N9	-11.68	107.96	113.80
26	BA	2451	A	C5-C6-N6	11.68	133.04	123.70
23	AW	42	A	N7-C8-N9	-11.68	107.96	113.80
26	BA	829	A	N7-C8-N9	-11.68	107.96	113.80
26	BA	340	A	N7-C8-N9	-11.68	107.96	113.80
26	BA	354	A	N7-C8-N9	-11.67	107.96	113.80
26	BA	1040	A	N7-C8-N9	-11.67	107.96	113.80
26	BA	2003	A	N7-C8-N9	-11.67	107.96	113.80
1	AA	414	A	N7-C8-N9	-11.67	107.96	113.80
1	AA	749	A	N7-C8-N9	-11.67	107.97	113.80
26	BA	990	A	N7-C8-N9	-11.67	107.97	113.80
26	BA	1354	A	N7-C8-N9	-11.67	107.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2761	A	N7-C8-N9	-11.67	107.97	113.80
26	BA	256	A	N7-C8-N9	-11.67	107.97	113.80
26	BA	310	A	N7-C8-N9	-11.67	107.97	113.80
26	BA	1786	A	N7-C8-N9	-11.67	107.97	113.80
26	BA	2590	A	N7-C8-N9	-11.67	107.97	113.80
1	AA	802	A	N7-C8-N9	-11.67	107.97	113.80
26	BA	1755	A	N7-C8-N9	-11.67	107.97	113.80
23	AW	41	A	N7-C8-N9	-11.66	107.97	113.80
26	BA	538	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	825	A	N7-C8-N9	-11.66	107.97	113.80
26	BA	42	A	N7-C8-N9	-11.66	107.97	113.80
26	BA	1237	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	681	A	N7-C8-N9	-11.66	107.97	113.80
26	BA	905	A	N7-C8-N9	-11.66	107.97	113.80
26	BA	2070	A	N7-C8-N9	-11.66	107.97	113.80
26	BA	2738	A	N7-C8-N9	-11.66	107.97	113.80
26	BA	1275	A	N7-C8-N9	-11.65	107.97	113.80
26	BA	1754	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	152	A	N7-C8-N9	-11.65	107.97	113.80
26	BA	1678	A	N7-C8-N9	-11.65	107.97	113.80
26	BA	1937	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	1248	A	N7-C8-N9	-11.65	107.97	113.80
26	BA	1566	A	N7-C8-N9	-11.65	107.97	113.80
26	BA	2534	A	N7-C8-N9	-11.65	107.97	113.80
26	BA	2829	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	695	A	N7-C8-N9	-11.65	107.98	113.80
1	AA	878	A	N7-C8-N9	-11.65	107.98	113.80
1	AA	1225	A	C5-C6-N6	11.65	133.02	123.70
1	AA	1394	A	N7-C8-N9	-11.65	107.98	113.80
26	BA	439	A	N7-C8-N9	-11.65	107.98	113.80
26	BA	1815	A	N7-C8-N9	-11.65	107.98	113.80
26	BA	2381	A	N7-C8-N9	-11.65	107.98	113.80
26	BA	2471	A	N7-C8-N9	-11.65	107.98	113.80
26	BA	2600	A	N7-C8-N9	-11.65	107.98	113.80
1	AA	978	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	241	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	1717	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	2281	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	2060	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	575	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	1089	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	2726	A	N7-C8-N9	-11.64	107.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2882	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	727	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	1308	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	2126	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	2657	A	N7-C8-N9	-11.64	107.98	113.80
26	BA	2851	A	N7-C8-N9	-11.64	107.98	113.80
1	AA	72	A	N7-C8-N9	-11.64	107.98	113.80
1	AA	687	A	N7-C8-N9	-11.64	107.98	113.80
1	AA	411	A	C5-C6-N6	11.63	133.01	123.70
1	AA	794	A	N7-C8-N9	-11.63	107.98	113.80
1	AA	1250	A	N7-C8-N9	-11.63	107.98	113.80
1	AA	1500	A	N7-C8-N9	-11.63	107.98	113.80
26	BA	89	A	N7-C8-N9	-11.63	107.98	113.80
26	BA	1569	A	N7-C8-N9	-11.63	107.98	113.80
26	BA	2679	A	N7-C8-N9	-11.63	107.98	113.80
26	BA	402	A	N7-C8-N9	-11.63	107.98	113.80
1	AA	366	A	N7-C8-N9	-11.63	107.98	113.80
26	BA	155	A	N7-C8-N9	-11.63	107.98	113.80
26	BA	1420	A	N7-C8-N9	-11.63	107.98	113.80
26	BA	1705	A	N7-C8-N9	-11.63	107.98	113.80
26	BA	1919	A	N7-C8-N9	-11.63	107.98	113.80
1	AA	320	A	N7-C8-N9	-11.63	107.98	113.80
1	AA	946	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	191	A	N7-C8-N9	-11.63	107.98	113.80
1	AA	1413	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	125	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	1134	A	N7-C8-N9	-11.63	107.98	113.80
26	BA	1143	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	1165	A	N7-C8-N9	-11.63	107.98	113.80
26	BA	1230	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	1254	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	1609	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	1722	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	2566	A	N7-C8-N9	-11.63	107.99	113.80
1	AA	655	A	N7-C8-N9	-11.63	107.99	113.80
1	AA	1201	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	1311	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	83	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	655	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	739	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	2288	A	N7-C8-N9	-11.63	107.99	113.80
26	BA	2503	A	N7-C8-N9	-11.62	107.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	253	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	338	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	1304	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	718	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	2270	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	66	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	1188	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	78	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	315	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	1302	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	2013	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	2406	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	2736	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	1272	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	1757	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	2033	A	C5-C6-N6	11.62	133.00	123.70
26	BA	2033	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	2883	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	16	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	223	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	861	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	945	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	1378	A	C5-C6-N6	11.62	132.99	123.70
1	AA	815	A	N7-C8-N9	-11.61	107.99	113.80
1	AA	1280	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	825	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	2135	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	38	A	N7-C8-N9	-11.61	107.99	113.80
26	BA	1641	A	N7-C8-N9	-11.61	107.99	113.80
26	BA	2241	A	N7-C8-N9	-11.62	107.99	113.80
26	BA	2377	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	101	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	1019	A	N7-C8-N9	-11.61	107.99	113.80
1	AA	1105	A	N7-C8-N9	-11.61	107.99	113.80
1	AA	1492	A	N7-C8-N9	-11.61	107.99	113.80
25	AY	35	A	N7-C8-N9	-11.61	107.99	113.80
26	BA	781	A	N7-C8-N9	-11.61	107.99	113.80
26	BA	2037	A	N7-C8-N9	-11.61	108.00	113.80
26	BA	2052	A	N7-C8-N9	-11.61	108.00	113.80
26	BA	2147	A	N7-C8-N9	-11.61	107.99	113.80
26	BA	2346	A	N7-C8-N9	-11.61	107.99	113.80
1	AA	1246	A	N7-C8-N9	-11.61	108.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	764	A	N7-C8-N9	-11.61	108.00	113.80
26	BA	1938	A	N7-C8-N9	-11.61	108.00	113.80
26	BA	2835	A	N7-C8-N9	-11.61	108.00	113.80
26	BA	483	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	676	A	N7-C8-N9	-11.61	108.00	113.80
25	AY	73	A	N7-C8-N9	-11.61	108.00	113.80
26	BA	608	A	N7-C8-N9	-11.61	108.00	113.80
26	BA	1366	A	N7-C8-N9	-11.61	108.00	113.80
26	BA	1630	A	C5-C6-N6	11.61	132.99	123.70
26	BA	2530	A	N7-C8-N9	-11.61	108.00	113.80
26	BA	1916	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	432	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	1213	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	349	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	452	A	C5-C6-N6	11.60	132.98	123.70
26	BA	507	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	2071	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	2298	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	2142	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	50	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	526	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	1503	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	541	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	983	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	2778	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	288	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	781	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	1147	A	C5-C6-N6	11.60	132.98	123.70
1	AA	1329	A	C5-C6-N6	11.60	132.98	123.70
26	BA	207	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	480	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	1057	A	N7-C8-N9	-11.60	108.00	113.80
26	BA	2117	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	139	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	309	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	49	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	324	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	878	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	1808	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	2108	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	160	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	1410	A	N7-C8-N9	-11.59	108.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1046	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	1551	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	1713	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	1749	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	1969	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	2119	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	2247	A	N7-C8-N9	-11.59	108.00	113.80
26	BA	2753	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	435	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	466	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	1257	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	1502	A	N7-C8-N9	-11.59	108.01	113.80
24	AX	9	A	N7-C8-N9	-11.59	108.01	113.80
25	AY	14	A	N7-C8-N9	-11.59	108.01	113.80
26	BA	1077	A	N7-C8-N9	-11.59	108.01	113.80
26	BA	1801	A	N7-C8-N9	-11.59	108.01	113.80
26	BA	2439	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	1101	A	N7-C8-N9	-11.59	108.01	113.80
26	BA	866	A	N7-C8-N9	-11.59	108.01	113.80
26	BA	1080	A	N7-C8-N9	-11.59	108.01	113.80
26	BA	1126	A	N7-C8-N9	-11.59	108.01	113.80
26	BA	1746	A	N7-C8-N9	-11.59	108.01	113.80
26	BA	2284	A	N7-C8-N9	-11.59	108.01	113.80
26	BA	2469	A	N7-C8-N9	-11.59	108.01	113.80
26	BA	2821	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	2893	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	383	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1285	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1483	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	637	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	979	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	1014	A	C5-C6-N6	11.58	132.97	123.70
26	BA	2335	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	2577	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	554	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1340	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	1987	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	497	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	668	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	1032	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	1503	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	1918	A	N7-C8-N9	-11.58	108.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2019	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	2358	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	2589	A	C5-C6-N6	11.58	132.96	123.70
1	AA	279	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	927	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	547	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	1470	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	1532	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	2173	A	N7-C8-N9	-11.58	108.01	113.80
26	BA	2560	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	55	A	N7-C8-N9	-11.57	108.01	113.80
1	AA	223	A	N7-C8-N9	-11.57	108.01	113.80
1	AA	1196	A	N7-C8-N9	-11.57	108.01	113.80
1	AA	303	A	N7-C8-N9	-11.57	108.01	113.80
1	AA	1318	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	947	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	176	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	347	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	492	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	996	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	1050	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	1677	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	1877	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	2670	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	2333	A	N7-C8-N9	-11.57	108.01	113.80
1	AA	10	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	734	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	1336	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	1502	A	N7-C8-N9	-11.57	108.01	113.80
1	AA	1428	A	N7-C8-N9	-11.57	108.02	113.80
25	AY	26	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	705	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	1054	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	1347	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	1654	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	2411	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	2665	A	N7-C8-N9	-11.57	108.01	113.80
26	BA	2154	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	2899	A	N7-C8-N9	-11.57	108.01	113.80
27	BB	109	A	N7-C8-N9	-11.57	108.01	113.80
1	AA	393	A	C5-C6-N6	11.57	132.95	123.70
1	AA	1434	A	N7-C8-N9	-11.57	108.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AV	15	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	144	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	270	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	621	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	1590	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	346	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	374	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	1073	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	1253	A	N7-C8-N9	-11.57	108.02	113.80
26	BA	2682	A	N7-C8-N9	-11.57	108.02	113.80
1	AA	465	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	535	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	1374	A	N7-C8-N9	-11.56	108.02	113.80
22	AV	21	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1593	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1952	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	449	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1286	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1591	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	2268	A	N7-C8-N9	-11.56	108.02	113.80
27	BB	46	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	327	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	747	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	782	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	1447	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	609	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1155	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1978	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	1256	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	217	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	454	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	749	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1307	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1698	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	2482	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	2654	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1403	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	2639	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	974	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	1117	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	391	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	602	A	N7-C8-N9	-11.56	108.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	909	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1175	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1848	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	2602	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	906	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	119	A	N7-C8-N9	-11.55	108.02	113.80
1	AA	199	A	N7-C8-N9	-11.55	108.02	113.80
1	AA	461	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	2170	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	1349	A	N7-C8-N9	-11.55	108.02	113.80
26	BA	1367	A	N7-C8-N9	-11.55	108.02	113.80
26	BA	1431	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	1735	A	N7-C8-N9	-11.55	108.02	113.80
26	BA	2198	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	2721	A	N7-C8-N9	-11.56	108.02	113.80
26	BA	693	A	N7-C8-N9	-11.55	108.02	113.80
26	BA	1214	A	N7-C8-N9	-11.55	108.02	113.80
26	BA	1932	A	N7-C8-N9	-11.55	108.02	113.80
26	BA	2461	A	N7-C8-N9	-11.55	108.02	113.80
26	BA	412	A	N7-C8-N9	-11.55	108.02	113.80
26	BA	1580	A	N7-C8-N9	-11.55	108.02	113.80
1	AA	28	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	622	A	C5-C6-N6	11.55	132.94	123.70
26	BA	272	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	616	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	2734	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	2800	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	325	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	453	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	1700	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	143	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	353	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	167	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	1008	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	1522	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	2030	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	2541	A	N7-C8-N9	-11.55	108.03	113.80
27	BB	66	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	2314	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	363	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	914	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	1289	A	N7-C8-N9	-11.55	108.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1819	A	N7-C8-N9	-11.55	108.03	113.80
26	BA	2448	A	N7-C8-N9	-11.55	108.03	113.80
27	BB	108	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	1204	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	1821	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	2810	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	250	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	900	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1067	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	221	A	N7-C8-N9	-11.54	108.03	113.80
27	BB	78	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	649	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	382	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	1247	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	1515	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	1853	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	1900	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	2088	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	2850	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	909	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	973	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	1111	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	2054	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	2435	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	151	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1287	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	104	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	1359	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	173	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	478	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	1085	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	1378	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	1689	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1333	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	2095	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	371	A	N7-C8-N9	-11.53	108.03	113.80
1	AA	768	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1111	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1229	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1275	A	N7-C8-N9	-11.53	108.03	113.80
1	AA	1518	A	N7-C8-N9	-11.54	108.03	113.80
26	BA	348	A	N7-C8-N9	-11.54	108.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	802	A	N7-C8-N9	-11.53	108.03	113.80
26	BA	1780	A	N7-C8-N9	-11.53	108.03	113.80
1	AA	80	A	N7-C8-N9	-11.53	108.03	113.80
1	AA	460	A	N7-C8-N9	-11.53	108.03	113.80
1	AA	1398	A	N7-C8-N9	-11.53	108.03	113.80
1	AA	1429	A	N7-C8-N9	-11.53	108.03	113.80
25	AY	6	A	N7-C8-N9	-11.53	108.03	113.80
26	BA	1504	A	N7-C8-N9	-11.53	108.03	113.80
26	BA	101	A	N7-C8-N9	-11.53	108.03	113.80
26	BA	1739	A	N7-C8-N9	-11.53	108.03	113.80
24	AX	21	A	N7-C8-N9	-11.53	108.03	113.80
1	AA	892	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	1441	A	N7-C8-N9	-11.53	108.04	113.80
24	AX	76	A	N7-C8-N9	-11.53	108.04	113.80
26	BA	819	A	N7-C8-N9	-11.53	108.03	113.80
26	BA	2660	A	N7-C8-N9	-11.53	108.03	113.80
26	BA	344	A	N7-C8-N9	-11.53	108.04	113.80
26	BA	432	A	N7-C8-N9	-11.53	108.04	113.80
26	BA	1858	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	65	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	167	A	N7-C8-N9	-11.53	108.04	113.80
24	AX	26	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	456	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	937	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	1251	A	N7-C8-N9	-11.53	108.04	113.80
26	BA	227	A	N7-C8-N9	-11.53	108.04	113.80
26	BA	460	A	N7-C8-N9	-11.53	108.04	113.80
26	BA	666	A	N7-C8-N9	-11.53	108.04	113.80
26	BA	936	A	N7-C8-N9	-11.53	108.04	113.80
26	BA	1803	A	N7-C8-N9	-11.53	108.04	113.80
26	BA	2059	A	N7-C8-N9	-11.53	108.04	113.80
26	BA	2352	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	1238	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1254	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	74	A	C5-C6-N6	11.52	132.92	123.70
1	AA	629	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1377	A	N7-C8-N9	-11.52	108.04	113.80
23	AW	26	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	428	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	917	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	1268	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	513	A	N7-C8-N9	-11.52	108.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1890	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	2705	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	2725	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	784	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1102	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1360	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1499	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	502	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	706	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	844	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	925	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	1353	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	1690	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	2750	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	1805	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	53	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	98	A	N7-C8-N9	-11.52	108.04	113.80
25	AY	21	A	N7-C8-N9	-11.52	108.04	113.80
25	AY	58	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	804	A	N7-C8-N9	-11.52	108.04	113.80
27	BB	58	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	415	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	918	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	1552	A	N7-C8-N9	-11.52	108.04	113.80
26	BA	2614	A	N7-C8-N9	-11.51	108.04	113.80
1	AA	777	A	N7-C8-N9	-11.51	108.04	113.80
1	AA	1274	A	N7-C8-N9	-11.51	108.04	113.80
23	AW	73	A	N7-C8-N9	-11.51	108.04	113.80
24	AX	41	A	N7-C8-N9	-11.51	108.04	113.80
26	BA	222	A	N7-C8-N9	-11.51	108.04	113.80
26	BA	482	A	N7-C8-N9	-11.51	108.04	113.80
26	BA	730	A	N7-C8-N9	-11.51	108.04	113.80
26	BA	1144	A	N7-C8-N9	-11.51	108.04	113.80
26	BA	1548	A	N7-C8-N9	-11.51	108.04	113.80
26	BA	1553	A	N7-C8-N9	-11.51	108.04	113.80
26	BA	1665	A	N7-C8-N9	-11.51	108.04	113.80
26	BA	1966	A	N7-C8-N9	-11.51	108.04	113.80
27	BB	119	A	N7-C8-N9	-11.51	108.04	113.80
26	BA	1321	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	172	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	274	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	792	A	N7-C8-N9	-11.51	108.05	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	860	A	N7-C8-N9	-11.51	108.05	113.80
25	AY	41	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	547	A	N7-C8-N9	-11.51	108.05	113.80
25	AY	69	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	95	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	1549	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	2005	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	2309	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	2814	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	171	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	165	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	1508	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	129	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	329	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	596	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	504	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	374	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	609	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	1413	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	1871	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	1912	A	N7-C8-N9	-11.51	108.05	113.80
26	BA	2516	A	N7-C8-N9	-11.51	108.05	113.80
27	BB	94	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	807	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	935	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	1081	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	1480	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	1433	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	501	A	N7-C8-N9	-11.50	108.05	113.80
22	AV	19	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	279	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	761	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1342	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1028	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1069	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1070	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1784	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1385	A	C5-C6-N6	11.50	132.90	123.70
1	AA	908	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	471	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	1082	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	1146	A	N7-C8-N9	-11.50	108.05	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	311	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	477	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	556	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2336	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	590	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1001	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2134	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	675	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	1437	A	N7-C8-N9	-11.50	108.05	113.80
23	AW	21	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	103	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	231	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	899	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1194	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1373	A	N7-C8-N9	-11.50	108.05	113.80
23	AW	38	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1205	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	1571	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2274	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2169	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2183	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2412	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2426	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2518	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2632	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2741	A	N7-C8-N9	-11.50	108.05	113.80
26	BA	2837	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	553	A	N7-C8-N9	-11.49	108.05	113.80
1	AA	790	A	N7-C8-N9	-11.49	108.05	113.80
1	AA	1150	A	C5-C6-N6	11.49	132.90	123.70
1	AA	1236	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	900	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	1597	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	2513	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	2764	A	N7-C8-N9	-11.49	108.05	113.80
1	AA	704	A	N7-C8-N9	-11.49	108.05	113.80
1	AA	718	A	N7-C8-N9	-11.49	108.05	113.80
1	AA	1446	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	470	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	1322	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	563	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	1244	A	N7-C8-N9	-11.49	108.05	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1434	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	1616	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	2700	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	2886	A	N7-C8-N9	-11.49	108.05	113.80
26	BA	21	A	N7-C8-N9	-11.49	108.06	113.80
26	BA	2634	A	N7-C8-N9	-11.49	108.06	113.80
26	BA	644	A	N7-C8-N9	-11.49	108.06	113.80
26	BA	2158	A	N7-C8-N9	-11.49	108.06	113.80
26	BA	2433	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	109	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	189	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	554	A	C5-C6-N6	11.49	132.89	123.70
1	AA	663	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	873	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	1022	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	1042	A	N7-C8-N9	-11.49	108.06	113.80
26	BA	742	A	N7-C8-N9	-11.49	108.06	113.80
26	BA	905	A	C5-C6-N6	11.49	132.89	123.70
26	BA	2311	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	19	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	77	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1145	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	614	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	1618	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	2340	A	N7-C8-N9	-11.48	108.06	113.80
27	BB	104	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	996	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	216	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	1169	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	1204	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	1668	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	573	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1000	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1012	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1046	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	199	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	789	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	877	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1150	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	44	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	911	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	1287	A	N7-C8-N9	-11.48	108.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1637	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	174	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	321	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	451	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	640	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1197	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	195	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	218	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	515	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	665	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1216	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	2176	A	N7-C8-N9	-11.48	108.06	113.80
26	BA	2322	A	C5-C6-N6	11.48	132.88	123.70
1	AA	26	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	179	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	373	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	630	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	975	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	1456	A	N7-C8-N9	-11.47	108.06	113.80
23	AW	58	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	1127	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	131	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	422	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	2211	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	59	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	130	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	635	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	746	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	969	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	1163	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	71	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	226	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	722	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	792	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	1156	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	1759	A	N7-C8-N9	-11.47	108.06	113.80
27	BB	101	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	1802	A	N7-C8-N9	-11.47	108.06	113.80
26	BA	2205	A	N7-C8-N9	-11.47	108.07	113.80
23	AW	66	A	N7-C8-N9	-11.47	108.07	113.80
26	BA	203	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	155	A	N7-C8-N9	-11.47	108.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	412	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	482	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	819	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	1170	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	352	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	1176	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	244	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	941	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	1020	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	1246	A	N7-C8-N9	-11.47	108.07	113.80
26	BA	1876	A	C5-C6-N6	11.46	132.87	123.70
26	BA	2366	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	32	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	336	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	560	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	28	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	661	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	1306	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	1396	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	1531	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	592	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	980	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	1701	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	529	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	821	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	1603	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	7	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	715	A	N7-C8-N9	-11.46	108.07	113.80
24	AX	14	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	431	A	N7-C8-N9	-11.46	108.07	113.80
25	AY	9	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	255	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	670	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	794	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	1090	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	1241	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	1650	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	574	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	938	A	N7-C8-N9	-11.45	108.07	113.80
1	AA	1110	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	1169	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	111	A	N7-C8-N9	-11.46	108.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	262	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	345	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	401	A	N7-C8-N9	-11.46	108.07	113.80
26	BA	472	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	959	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	1129	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	1927	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	2014	A	N7-C8-N9	-11.46	108.07	113.80
27	BB	34	A	C5-C6-N6	11.46	132.86	123.70
26	BA	1151	A	N7-C8-N9	-11.45	108.07	113.80
1	AA	712	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	1465	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	63	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	156	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	190	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	508	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	1711	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	2453	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	1847	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	2199	A	N7-C8-N9	-11.45	108.07	113.80
26	BA	2727	A	N7-C8-N9	-11.45	108.07	113.80
1	AA	262	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	533	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	702	A	N7-C8-N9	-11.45	108.08	113.80
25	AY	66	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	1098	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	1528	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	309	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	750	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	988	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	1545	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	1937	A	C5-C6-N6	11.45	132.86	123.70
26	BA	2792	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	344	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	600	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	648	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	716	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	19	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	964	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	699	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	1477	A	N7-C8-N9	-11.45	108.08	113.80
26	BA	1610	A	N7-C8-N9	-11.45	108.08	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2418	A	C5-C6-N6	11.45	132.86	123.70
1	AA	1157	A	N7-C8-N9	-11.44	108.08	113.80
23	AW	31	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	918	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1271	A	N7-C8-N9	-11.44	108.08	113.80
24	AX	23	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	146	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	172	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	282	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	368	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	522	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	621	A	C5-C6-N6	11.44	132.85	123.70
26	BA	1635	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	1544	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	282	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1180	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1513	A	N7-C8-N9	-11.44	108.08	113.80
23	AW	42	A	C5-C6-N6	11.44	132.85	123.70
26	BA	91	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	94	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	676	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	2856	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	278	A	N3-C4-C5	-11.44	118.79	126.80
27	BB	39	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	622	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	968	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1130	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	182	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	2749	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1171	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	197	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	928	A	N7-C8-N9	-11.44	108.08	113.80
26	BA	1419	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	228	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	298	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	816	A	N7-C8-N9	-11.43	108.08	113.80
27	BB	50	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	1350	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	1476	A	N7-C8-N9	-11.43	108.08	113.80
26	BA	6	A	N7-C8-N9	-11.43	108.08	113.80
26	BA	160	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	1431	A	N7-C8-N9	-11.43	108.08	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	447	A	N7-C8-N9	-11.43	108.08	113.80
26	BA	627	A	N7-C8-N9	-11.43	108.08	113.80
26	BA	643	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	642	A	N7-C8-N9	-11.43	108.09	113.80
26	BA	626	A	N7-C8-N9	-11.43	108.09	113.80
26	BA	1027	A	N7-C8-N9	-11.43	108.09	113.80
26	BA	1040	A	C5-C6-N6	11.43	132.84	123.70
26	BA	1626	A	N7-C8-N9	-11.43	108.09	113.80
26	BA	1679	A	N7-C8-N9	-11.43	108.08	113.80
26	BA	1998	A	N7-C8-N9	-11.43	108.09	113.80
26	BA	1572	A	N7-C8-N9	-11.43	108.09	113.80
26	BA	2227	A	N7-C8-N9	-11.43	108.09	113.80
26	BA	2587	A	N7-C8-N9	-11.43	108.09	113.80
26	BA	14	A	N7-C8-N9	-11.43	108.09	113.80
26	BA	2675	A	N7-C8-N9	-11.43	108.09	113.80
1	AA	382	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	1375	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	64	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	599	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	2278	A	N7-C8-N9	-11.42	108.09	113.80
27	BB	115	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	33	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	743	A	N7-C8-N9	-11.42	108.09	113.80
23	AW	59	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	753	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	1213	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	1327	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	171	A	C5-C6-N6	11.42	132.84	123.70
1	AA	313	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	595	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	706	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	864	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	907	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	1468	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	1493	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	126	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	503	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	1453	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	2266	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	219	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	356	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	787	A	N7-C8-N9	-11.42	108.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2733	A	N7-C8-N9	-11.42	108.09	113.80
24	AX	3	A	N7-C8-N9	-11.42	108.09	113.80
24	AX	24	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	1095	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	1586	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	1785	A	C5-C6-N6	11.42	132.83	123.70
26	BA	1829	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	2273	A	N7-C8-N9	-11.42	108.09	113.80
26	BA	2432	A	N7-C8-N9	-11.42	108.09	113.80
27	BB	53	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	81	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	181	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	2154	A	C5-C6-N6	11.41	132.83	123.70
22	AV	20	A	N7-C8-N9	-11.41	108.09	113.80
23	AW	9	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	1596	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	2565	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	729	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	1789	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	1885	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	393	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	342	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	1505	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	1970	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	2077	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	2476	A	N7-C8-N9	-11.41	108.09	113.80
26	BA	2900	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	1519	A	N7-C8-N9	-11.41	108.10	113.80
26	BA	423	A	N7-C8-N9	-11.41	108.10	113.80
26	BA	1029	A	N7-C8-N9	-11.41	108.10	113.80
26	BA	1579	A	N7-C8-N9	-11.41	108.10	113.80
26	BA	1854	A	N7-C8-N9	-11.41	108.10	113.80
26	BA	1048	A	N7-C8-N9	-11.41	108.10	113.80
26	BA	1889	A	N7-C8-N9	-11.41	108.10	113.80
26	BA	2740	A	N7-C8-N9	-11.41	108.10	113.80
1	AA	487	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	607	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	845	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	5	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	849	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	1067	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	1672	A	N7-C8-N9	-11.40	108.10	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	696	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	1103	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	2434	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	270	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	431	A	C5-C6-N6	11.40	132.82	123.70
1	AA	532	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	213	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	411	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	621	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	56	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	2212	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	2711	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	559	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	919	A	N7-C8-N9	-11.40	108.10	113.80
23	AW	23	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	322	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	1328	A	N7-C8-N9	-11.40	108.10	113.80
26	BA	1395	A	N7-C8-N9	-11.40	108.10	113.80
23	AW	69	A	N7-C8-N9	-11.39	108.10	113.80
26	BA	582	A	N7-C8-N9	-11.39	108.10	113.80
26	BA	735	A	N7-C8-N9	-11.39	108.10	113.80
26	BA	1000	A	N7-C8-N9	-11.39	108.10	113.80
26	BA	152	A	N7-C8-N9	-11.39	108.10	113.80
26	BA	1744	A	N7-C8-N9	-11.39	108.10	113.80
27	BB	99	A	N7-C8-N9	-11.39	108.10	113.80
1	AA	162	A	N7-C8-N9	-11.39	108.11	113.80
1	AA	493	A	N7-C8-N9	-11.39	108.11	113.80
25	AY	23	A	N7-C8-N9	-11.39	108.10	113.80
26	BA	2191	A	N7-C8-N9	-11.39	108.10	113.80
26	BA	1494	A	N7-C8-N9	-11.39	108.11	113.80
26	BA	2748	A	N7-C8-N9	-11.39	108.10	113.80
1	AA	448	A	N7-C8-N9	-11.39	108.11	113.80
26	BA	685	A	N7-C8-N9	-11.39	108.11	113.80
26	BA	716	A	N7-C8-N9	-11.39	108.11	113.80
26	BA	1525	A	N7-C8-N9	-11.39	108.11	113.80
26	BA	782	A	N7-C8-N9	-11.39	108.11	113.80
26	BA	1274	A	N7-C8-N9	-11.39	108.11	113.80
26	BA	1981	A	N7-C8-N9	-11.39	108.11	113.80
26	BA	2706	A	N7-C8-N9	-11.39	108.11	113.80
1	AA	1507	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	300	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	1189	A	N7-C8-N9	-11.38	108.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1640	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	1787	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	2097	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	780	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1035	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1036	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1319	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	119	A	C5-C6-N6	11.38	132.81	123.70
26	BA	586	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	1264	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	2015	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	1276	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	1785	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	2225	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	520	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	74	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	238	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	364	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1288	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1430	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	689	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	896	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	1285	A	N7-C8-N9	-11.38	108.11	113.80
27	BB	15	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	195	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	498	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1044	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	299	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	721	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	1632	A	N7-C8-N9	-11.38	108.11	113.80
26	BA	1284	A	N7-C8-N9	-11.37	108.11	113.80
26	BA	1936	A	N7-C8-N9	-11.37	108.11	113.80
26	BA	415	A	N7-C8-N9	-11.37	108.11	113.80
26	BA	2042	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	205	A	N7-C8-N9	-11.37	108.12	113.80
1	AA	523	A	N7-C8-N9	-11.37	108.11	113.80
26	BA	2425	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	572	A	N7-C8-N9	-11.37	108.12	113.80
1	AA	1261	A	N7-C8-N9	-11.37	108.11	113.80
22	AV	17	A	N7-C8-N9	-11.37	108.11	113.80
26	BA	756	A	N7-C8-N9	-11.37	108.11	113.80
26	BA	820	A	N7-C8-N9	-11.37	108.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	76	A	N7-C8-N9	-11.37	108.12	113.80
26	BA	751	A	N7-C8-N9	-11.37	108.12	113.80
26	BA	1039	A	N7-C8-N9	-11.37	108.11	113.80
26	BA	2873	A	N7-C8-N9	-11.37	108.11	113.80
26	BA	2872	A	N7-C8-N9	-11.37	108.12	113.80
1	AA	71	A	N7-C8-N9	-11.37	108.12	113.80
1	AA	1534	A	N7-C8-N9	-11.37	108.12	113.80
26	BA	943	A	N7-C8-N9	-11.37	108.12	113.80
26	BA	1260	A	N7-C8-N9	-11.37	108.12	113.80
26	BA	1009	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	1133	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	2781	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	2826	A	N7-C8-N9	-11.37	108.12	113.80
1	AA	3	A	N7-C8-N9	-11.36	108.12	113.80
1	AA	579	A	N7-C8-N9	-11.36	108.12	113.80
1	AA	1269	A	N7-C8-N9	-11.36	108.12	113.80
1	AA	1299	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	892	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	1384	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	1608	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	1977	A	N7-C8-N9	-11.36	108.12	113.80
1	AA	766	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	972	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	2376	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	2468	A	N7-C8-N9	-11.36	108.12	113.80
26	BA	631	A	N7-C8-N9	-11.35	108.12	113.80
26	BA	2799	A	N7-C8-N9	-11.35	108.12	113.80
1	AA	1191	A	N7-C8-N9	-11.35	108.12	113.80
26	BA	118	A	N7-C8-N9	-11.35	108.12	113.80
26	BA	2171	A	N7-C8-N9	-11.35	108.12	113.80
26	BA	2497	A	N7-C8-N9	-11.35	108.12	113.80
1	AA	151	A	C5-C6-N6	11.35	132.78	123.70
1	AA	1170	A	C5-C6-N6	11.35	132.78	123.70
26	BA	920	A	N7-C8-N9	-11.35	108.12	113.80
26	BA	1469	A	N7-C8-N9	-11.35	108.12	113.80
26	BA	2635	A	N7-C8-N9	-11.35	108.12	113.80
26	BA	2860	A	N7-C8-N9	-11.35	108.12	113.80
26	BA	2887	A	N7-C8-N9	-11.35	108.12	113.80
26	BA	2451	A	N7-C8-N9	-11.35	108.13	113.80
26	BA	1590	A	C5-C6-N6	11.35	132.78	123.70
26	BA	429	A	N7-C8-N9	-11.35	108.13	113.80
1	AA	1363	A	N7-C8-N9	-11.34	108.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	362	A	N7-C8-N9	-11.34	108.13	113.80
26	BA	654	A	N7-C8-N9	-11.34	108.13	113.80
26	BA	2369	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	539	A	N7-C8-N9	-11.34	108.13	113.80
26	BA	715	A	N7-C8-N9	-11.34	108.13	113.80
26	BA	1745	A	N7-C8-N9	-11.34	108.13	113.80
26	BA	2868	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	306	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	1004	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	1093	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	1346	A	N7-C8-N9	-11.34	108.13	113.80
26	BA	354	A	C5-C6-N6	11.34	132.77	123.70
26	BA	1269	A	N7-C8-N9	-11.34	108.13	113.80
26	BA	1392	A	N7-C8-N9	-11.33	108.13	113.80
26	BA	2459	A	N7-C8-N9	-11.33	108.13	113.80
26	BA	294	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	149	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	766	A	C5-C6-N6	11.33	132.76	123.70
1	AA	831	A	N7-C8-N9	-11.33	108.14	113.80
26	BA	793	A	N7-C8-N9	-11.33	108.14	113.80
27	BB	59	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	182	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	192	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	889	A	C5-C6-N6	11.33	132.76	123.70
1	AA	994	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	1092	A	N7-C8-N9	-11.33	108.14	113.80
26	BA	233	A	N7-C8-N9	-11.33	108.14	113.80
26	BA	1383	A	N7-C8-N9	-11.33	108.14	113.80
26	BA	2809	A	N7-C8-N9	-11.33	108.14	113.80
26	BA	2407	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	1227	A	N7-C8-N9	-11.32	108.14	113.80
26	BA	13	A	N7-C8-N9	-11.32	108.14	113.80
26	BA	1495	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	478	A	N7-C8-N9	-11.32	108.14	113.80
26	BA	1439	A	N7-C8-N9	-11.32	108.14	113.80
26	BA	1762	A	N7-C8-N9	-11.32	108.14	113.80
27	BB	45	A	N7-C8-N9	-11.32	108.14	113.80
26	BA	443	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	1016	A	N7-C8-N9	-11.32	108.14	113.80
26	BA	1496	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	1508	A	N7-C8-N9	-11.32	108.14	113.80
26	BA	668	A	C5-C6-N6	11.32	132.75	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1387	A	N7-C8-N9	-11.32	108.14	113.80
26	BA	2564	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	300	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	825	A	C5-C6-N6	11.31	132.75	123.70
26	BA	2386	A	N7-C8-N9	-11.31	108.14	113.80
26	BA	2764	A	C5-C6-N6	11.31	132.75	123.70
1	AA	452	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	161	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	814	A	N7-C8-N9	-11.31	108.14	113.80
26	BA	2879	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	236	A	N7-C8-N9	-11.31	108.15	113.80
26	BA	42	A	C5-C6-N6	11.31	132.75	123.70
26	BA	330	A	N7-C8-N9	-11.31	108.15	113.80
26	BA	2094	A	N7-C8-N9	-11.31	108.15	113.80
1	AA	179	A	C5-C6-N6	11.30	132.74	123.70
1	AA	608	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	1362	A	N7-C8-N9	-11.30	108.15	113.80
26	BA	514	A	N7-C8-N9	-11.31	108.15	113.80
26	BA	863	A	N7-C8-N9	-11.31	108.15	113.80
26	BA	1393	A	N7-C8-N9	-11.31	108.15	113.80
26	BA	675	A	N7-C8-N9	-11.30	108.15	113.80
26	BA	1772	A	C5-C6-N6	11.30	132.74	123.70
26	BA	752	A	N7-C8-N9	-11.30	108.15	113.80
26	BA	2108	A	C5-C6-N6	11.30	132.74	123.70
26	BA	1084	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	389	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	1227	A	C5-C6-N6	11.30	132.74	123.70
26	BA	1155	A	C5-C6-N6	11.30	132.74	123.70
26	BA	2531	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	243	A	C5-C6-N6	11.29	132.74	123.70
1	AA	430	A	N7-C8-N9	-11.29	108.15	113.80
1	AA	468	A	N7-C8-N9	-11.29	108.15	113.80
26	BA	2009	A	C5-C6-N6	11.29	132.73	123.70
1	AA	1339	A	N7-C8-N9	-11.29	108.16	113.80
26	BA	613	A	N7-C8-N9	-11.29	108.16	113.80
26	BA	2247	A	C5-C6-N6	11.29	132.73	123.70
1	AA	1324	A	N7-C8-N9	-11.29	108.16	113.80
26	BA	1304	A	C5-C6-N6	11.29	132.73	123.70
26	BA	1545	A	C5-C6-N6	11.29	132.73	123.70
26	BA	2020	A	N7-C8-N9	-11.29	108.16	113.80
1	AA	309	A	C5-C6-N6	11.28	132.72	123.70
1	AA	1021	A	N7-C8-N9	-11.28	108.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	572	A	N7-C8-N9	-11.28	108.16	113.80
26	BA	1433	A	N7-C8-N9	-11.28	108.16	113.80
1	AA	196	A	N7-C8-N9	-11.28	108.16	113.80
1	AA	1000	A	C5-C6-N6	11.28	132.72	123.70
26	BA	38	A	C5-C6-N6	11.28	132.72	123.70
26	BA	404	A	N7-C8-N9	-11.28	108.16	113.80
1	AA	1410	A	C5-C6-N6	11.28	132.72	123.70
26	BA	457	A	C5-C6-N6	11.28	132.72	123.70
26	BA	743	A	N7-C8-N9	-11.28	108.16	113.80
26	BA	1755	A	C5-C6-N6	11.28	132.72	123.70
26	BA	1953	A	N7-C8-N9	-11.28	108.16	113.80
26	BA	800	A	C5-C6-N6	11.28	132.72	123.70
26	BA	2114	A	N3-C4-C5	-11.28	118.91	126.80
26	BA	2071	A	C5-C6-N6	11.27	132.72	123.70
1	AA	728	A	N7-C8-N9	-11.27	108.16	113.80
27	BB	78	A	C5-C6-N6	11.27	132.72	123.70
1	AA	958	A	N7-C8-N9	-11.27	108.17	113.80
26	BA	2513	A	C5-C6-N6	11.27	132.72	123.70
26	BA	2547	A	N7-C8-N9	-11.27	108.16	113.80
1	AA	665	A	C5-C6-N6	11.27	132.72	123.70
1	AA	983	A	N3-C4-C5	-11.27	118.91	126.80
1	AA	1151	A	C5-C6-N6	11.27	132.72	123.70
26	BA	1096	A	N7-C8-N9	-11.27	108.17	113.80
26	BA	1226	A	N7-C8-N9	-11.27	108.17	113.80
26	BA	2090	A	C5-C6-N6	11.27	132.71	123.70
1	AA	496	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	1418	A	N7-C8-N9	-11.26	108.17	113.80
26	BA	984	A	N7-C8-N9	-11.26	108.17	113.80
26	BA	10	A	N7-C8-N9	-11.26	108.17	113.80
26	BA	825	A	C5-C6-N6	11.26	132.71	123.70
26	BA	1365	A	N7-C8-N9	-11.26	108.17	113.80
26	BA	2184	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	499	A	C5-C6-N6	11.26	132.71	123.70
1	AA	681	A	C5-C6-N6	11.26	132.71	123.70
26	BA	975	A	N7-C8-N9	-11.26	108.17	113.80
26	BA	2813	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	1219	A	N7-C8-N9	-11.26	108.17	113.80
26	BA	1809	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	510	A	N7-C8-N9	-11.26	108.17	113.80
26	BA	53	A	N7-C8-N9	-11.25	108.17	113.80
26	BA	1308	A	C5-C6-N6	11.25	132.70	123.70
26	BA	1598	A	N7-C8-N9	-11.25	108.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1614	A	N7-C8-N9	-11.25	108.17	113.80
1	AA	1014	A	N7-C8-N9	-11.25	108.17	113.80
26	BA	1204	A	C5-C6-N6	11.25	132.70	123.70
1	AA	2	A	N7-C8-N9	-11.25	108.18	113.80
26	BA	2566	A	C5-C6-N6	11.25	132.70	123.70
1	AA	253	A	C5-C6-N6	11.25	132.70	123.70
26	BA	2163	A	N7-C8-N9	-11.25	108.18	113.80
26	BA	2600	A	C5-C6-N6	11.25	132.70	123.70
26	BA	1928	A	N7-C8-N9	-11.24	108.18	113.80
27	BB	57	A	N7-C8-N9	-11.24	108.18	113.80
26	BA	1262	A	N7-C8-N9	-11.24	108.18	113.80
26	BA	2820	A	N7-C8-N9	-11.24	108.18	113.80
1	AA	1248	A	C5-C6-N6	11.24	132.69	123.70
1	AA	1357	A	N7-C8-N9	-11.23	108.18	113.80
1	AA	1437	A	C5-C6-N6	11.23	132.69	123.70
26	BA	53	A	C5-C6-N6	11.23	132.69	123.70
26	BA	1165	A	C5-C6-N6	11.23	132.69	123.70
26	BA	1010	A	N7-C8-N9	-11.23	108.18	113.80
26	BA	2378	A	N7-C8-N9	-11.23	108.18	113.80
26	BA	2757	A	N7-C8-N9	-11.23	108.19	113.80
26	BA	1086	A	N7-C8-N9	-11.23	108.19	113.80
1	AA	195	A	C5-C6-N6	11.22	132.68	123.70
26	BA	1783	A	N7-C8-N9	-11.22	108.19	113.80
26	BA	1791	A	N7-C8-N9	-11.22	108.19	113.80
26	BA	2080	A	N7-C8-N9	-11.22	108.19	113.80
1	AA	131	A	C5-C6-N6	11.22	132.67	123.70
26	BA	204	A	C5-C6-N6	11.22	132.68	123.70
26	BA	1057	A	C5-C6-N6	11.21	132.67	123.70
26	BA	2450	A	N7-C8-N9	-11.21	108.19	113.80
26	BA	2590	A	C5-C6-N6	11.21	132.67	123.70
26	BA	2761	A	C5-C6-N6	11.21	132.67	123.70
1	AA	782	A	C5-C6-N6	11.21	132.67	123.70
26	BA	2317	A	N7-C8-N9	-11.21	108.19	113.80
26	BA	1593	A	C5-C6-N6	11.21	132.67	123.70
26	BA	2134	A	C5-C6-N6	11.21	132.67	123.70
26	BA	981	A	N7-C8-N9	-11.21	108.20	113.80
1	AA	44	A	C5-C6-N6	11.21	132.66	123.70
26	BA	161	A	N7-C8-N9	-11.21	108.20	113.80
1	AA	190	A	N7-C8-N9	-11.20	108.20	113.80
1	AA	502	A	N7-C8-N9	-11.20	108.20	113.80
26	BA	1088	A	N7-C8-N9	-11.20	108.20	113.80
1	AA	1238	A	C5-C6-N6	11.20	132.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1427	A	C5-C6-N6	11.20	132.66	123.70
27	BB	29	A	N7-C8-N9	-11.20	108.20	113.80
1	AA	1368	A	C5-C6-N6	11.20	132.66	123.70
26	BA	111	A	C5-C6-N6	11.20	132.66	123.70
26	BA	783	A	C5-C6-N6	11.19	132.65	123.70
27	BB	29	A	C5-C6-N6	11.19	132.65	123.70
26	BA	207	A	C5-C6-N6	11.19	132.65	123.70
26	BA	1502	A	C5-C6-N6	11.19	132.65	123.70
26	BA	2736	A	C5-C6-N6	11.19	132.65	123.70
1	AA	80	A	C5-C6-N6	11.19	132.65	123.70
26	BA	1583	A	N7-C8-N9	-11.19	108.21	113.80
26	BA	1001	A	C5-C6-N6	11.19	132.65	123.70
1	AA	349	A	C5-C6-N6	11.18	132.65	123.70
1	AA	648	A	C5-C6-N6	11.18	132.65	123.70
26	BA	1810	A	N7-C8-N9	-11.18	108.21	113.80
1	AA	129	A	C5-C6-N6	11.18	132.64	123.70
1	AA	978	A	C5-C6-N6	11.18	132.64	123.70
26	BA	574	A	C5-C6-N6	11.18	132.64	123.70
1	AA	865	A	N7-C8-N9	-11.18	108.21	113.80
26	BA	430	A	N7-C8-N9	-11.18	108.21	113.80
26	BA	1652	A	C5-C6-N6	11.17	132.64	123.70
1	AA	1080	A	N7-C8-N9	-11.17	108.22	113.80
26	BA	52	A	N7-C8-N9	-11.17	108.22	113.80
26	BA	2019	A	C5-C6-N6	11.17	132.64	123.70
1	AA	1229	A	C5-C6-N6	11.17	132.63	123.70
26	BA	845	A	N7-C8-N9	-11.17	108.22	113.80
26	BA	1535	A	N7-C8-N9	-11.17	108.22	113.80
26	BA	1872	A	N7-C8-N9	-11.17	108.22	113.80
1	AA	459	A	N7-C8-N9	-11.16	108.22	113.80
1	AA	1332	A	N7-C8-N9	-11.16	108.22	113.80
26	BA	1821	A	C5-C6-N6	11.16	132.63	123.70
26	BA	2632	A	C5-C6-N6	11.16	132.63	123.70
26	BA	1676	A	N7-C8-N9	-11.16	108.22	113.80
26	BA	1953	A	C5-C6-N6	11.16	132.63	123.70
26	BA	2176	A	C5-C6-N6	11.16	132.63	123.70
26	BA	371	A	C5-C6-N6	11.16	132.63	123.70
26	BA	2225	A	C5-C6-N6	11.16	132.63	123.70
26	BA	933	A	N7-C8-N9	-11.16	108.22	113.80
26	BA	1413	A	C5-C6-N6	11.16	132.63	123.70
26	BA	2765	A	N7-C8-N9	-11.16	108.22	113.80
1	AA	1204	A	C5-C6-N6	11.16	132.62	123.70
26	BA	156	A	C5-C6-N6	11.16	132.63	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1490	A	N7-C8-N9	-11.16	108.22	113.80
26	BA	1749	A	C5-C6-N6	11.16	132.63	123.70
1	AA	1333	A	C5-C6-N6	11.15	132.62	123.70
26	BA	2823	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	878	A	C5-C6-N6	11.15	132.62	123.70
26	BA	2005	A	C5-C6-N6	11.15	132.62	123.70
26	BA	2058	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	1225	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	1513	A	C5-C6-N6	11.15	132.62	123.70
26	BA	241	A	C5-C6-N6	11.15	132.62	123.70
26	BA	2757	A	C5-C6-N6	11.14	132.62	123.70
1	AA	10	A	C5-C6-N6	11.14	132.61	123.70
1	AA	923	A	N7-C8-N9	-11.14	108.23	113.80
1	AA	1289	A	C5-C6-N6	11.14	132.62	123.70
26	BA	1503	A	C5-C6-N6	11.14	132.61	123.70
26	BA	833	A	N7-C8-N9	-11.14	108.23	113.80
26	BA	2392	A	C5-C6-N6	11.13	132.61	123.70
26	BA	2435	A	C5-C6-N6	11.13	132.61	123.70
1	AA	533	A	C5-C6-N6	11.13	132.61	123.70
26	BA	165	A	C5-C6-N6	11.13	132.61	123.70
27	BB	73	A	N7-C8-N9	-11.13	108.23	113.80
26	BA	155	A	C5-C6-N6	11.13	132.60	123.70
1	AA	749	A	C5-C6-N6	11.13	132.60	123.70
26	BA	127	A	N7-C8-N9	-11.13	108.24	113.80
26	BA	2101	A	C5-C6-N6	11.13	132.60	123.70
26	BA	2381	A	C5-C6-N6	11.13	132.60	123.70
26	BA	2450	A	C5-C6-N6	11.13	132.60	123.70
1	AA	1082	A	C5-C6-N6	11.12	132.60	123.70
1	AA	1155	A	C5-C6-N6	11.12	132.60	123.70
26	BA	783	A	N7-C8-N9	-11.12	108.24	113.80
26	BA	1262	A	C5-C6-N6	11.12	132.60	123.70
26	BA	1987	A	C5-C6-N6	11.12	132.60	123.70
26	BA	2453	A	C5-C6-N6	11.12	132.60	123.70
1	AA	509	A	N7-C8-N9	-11.12	108.24	113.80
1	AA	573	A	C5-C6-N6	11.12	132.59	123.70
26	BA	983	A	C5-C6-N6	11.12	132.60	123.70
26	BA	84	A	C5-C6-N6	11.12	132.59	123.70
26	BA	802	A	C5-C6-N6	11.12	132.59	123.70
26	BA	1803	A	C5-C6-N6	11.12	132.59	123.70
26	BA	2388	A	C5-C6-N6	11.12	132.60	123.70
26	BA	2899	A	C5-C6-N6	11.12	132.60	123.70
1	AA	182	A	C5-C6-N6	11.12	132.59	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1005	A	N7-C8-N9	-11.12	108.24	113.80
26	BA	918	A	C5-C6-N6	11.12	132.59	123.70
26	BA	1960	A	C5-C6-N6	11.12	132.59	123.70
26	BA	1515	A	C5-C6-N6	11.11	132.59	123.70
26	BA	2241	A	C5-C6-N6	11.11	132.59	123.70
26	BA	460	A	C5-C6-N6	11.11	132.59	123.70
26	BA	1086	A	C5-C6-N6	11.11	132.59	123.70
26	BA	2882	A	C5-C6-N6	11.11	132.59	123.70
1	AA	327	A	C5-C6-N6	11.11	132.59	123.70
1	AA	139	A	C5-C6-N6	11.11	132.58	123.70
26	BA	2298	A	C5-C6-N6	11.11	132.58	123.70
1	AA	336	A	C5-C6-N6	11.10	132.58	123.70
26	BA	347	A	C5-C6-N6	11.10	132.58	123.70
26	BA	529	A	C5-C6-N6	11.10	132.58	123.70
26	BA	586	A	C5-C6-N6	11.10	132.58	123.70
26	BA	676	A	C5-C6-N6	11.10	132.58	123.70
26	BA	1286	A	C5-C6-N6	11.10	132.58	123.70
26	BA	1668	A	C5-C6-N6	11.10	132.58	123.70
26	BA	973	A	C5-C6-N6	11.10	132.58	123.70
26	BA	1901	A	N7-C8-N9	-11.10	108.25	113.80
26	BA	2766	A	N7-C8-N9	-11.10	108.25	113.80
1	AA	101	A	C5-C6-N6	11.10	132.58	123.70
26	BA	538	A	C5-C6-N6	11.10	132.58	123.70
1	AA	977	A	N7-C8-N9	-11.10	108.25	113.80
26	BA	849	A	C5-C6-N6	11.10	132.58	123.70
1	AA	26	A	C5-C6-N6	11.09	132.57	123.70
1	AA	959	A	N7-C8-N9	-11.09	108.25	113.80
1	AA	969	A	C5-C6-N6	11.09	132.57	123.70
26	BA	1246	A	C5-C6-N6	11.09	132.57	123.70
26	BA	2565	A	C5-C6-N6	11.09	132.57	123.70
26	BA	2829	A	C5-C6-N6	11.09	132.57	123.70
1	AA	456	A	C5-C6-N6	11.09	132.57	123.70
1	AA	66	A	C5-C6-N6	11.09	132.57	123.70
26	BA	480	A	C5-C6-N6	11.09	132.57	123.70
26	BA	1194	A	C5-C6-N6	11.09	132.57	123.70
26	BA	2015	A	C5-C6-N6	11.09	132.57	123.70
1	AA	149	A	C5-C6-N6	11.09	132.57	123.70
1	AA	915	A	C5-C6-N6	11.09	132.57	123.70
26	BA	73	A	N7-C8-N9	-11.09	108.26	113.80
26	BA	2469	A	C5-C6-N6	11.09	132.57	123.70
26	BA	2051	A	N7-C8-N9	-11.08	108.26	113.80
1	AA	1428	A	C5-C6-N6	11.08	132.56	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	910	A	C5-C6-N6	11.08	132.56	123.70
26	BA	1347	A	C5-C6-N6	11.08	132.56	123.70
26	BA	1794	A	C5-C6-N6	11.08	132.56	123.70
26	BA	2639	A	C5-C6-N6	11.08	132.56	123.70
1	AA	802	A	C5-C6-N6	11.08	132.56	123.70
26	BA	514	A	C5-C6-N6	11.08	132.56	123.70
26	BA	1901	A	C5-C6-N6	11.08	132.56	123.70
23	AW	41	A	C5-C6-N6	11.08	132.56	123.70
26	BA	1586	A	C5-C6-N6	11.07	132.56	123.70
1	AA	313	A	C5-C6-N6	11.07	132.56	123.70
1	AA	583	A	C5-C6-N6	11.07	132.56	123.70
26	BA	981	A	C5-C6-N6	11.07	132.56	123.70
23	AW	9	A	C5-C6-N6	11.07	132.56	123.70
23	AW	69	A	C5-C6-N6	11.07	132.56	123.70
1	AA	816	A	C5-C6-N6	11.07	132.56	123.70
1	AA	263	A	C5-C6-N6	11.07	132.55	123.70
26	BA	466	A	C5-C6-N6	11.07	132.55	123.70
1	AA	1055	A	C5-C6-N6	11.07	132.55	123.70
1	AA	1349	A	C5-C6-N6	11.07	132.55	123.70
1	AA	498	A	C5-C6-N6	11.06	132.55	123.70
1	AA	1413	A	C5-C6-N6	11.06	132.55	123.70
26	BA	861	A	C5-C6-N6	11.06	132.55	123.70
26	BA	346	A	C5-C6-N6	11.06	132.55	123.70
26	BA	1866	A	N7-C8-N9	-11.06	108.27	113.80
26	BA	2062	A	N7-C8-N9	-11.06	108.27	113.80
26	BA	2572	A	C5-C6-N6	11.06	132.55	123.70
26	BA	104	A	C5-C6-N6	11.06	132.55	123.70
26	BA	1237	A	C5-C6-N6	11.06	132.55	123.70
26	BA	2734	A	C5-C6-N6	11.06	132.55	123.70
26	BA	196	A	N7-C8-N9	-11.06	108.27	113.80
1	AA	263	A	N7-C8-N9	-11.06	108.27	113.80
26	BA	1268	A	C5-C6-N6	11.06	132.55	123.70
27	BB	52	A	C5-C6-N6	11.06	132.55	123.70
1	AA	374	A	C5-C6-N6	11.05	132.54	123.70
1	AA	1311	A	C5-C6-N6	11.05	132.54	123.70
26	BA	217	A	C5-C6-N6	11.06	132.54	123.70
26	BA	829	A	C5-C6-N6	11.06	132.54	123.70
26	BA	2868	A	C5-C6-N6	11.06	132.54	123.70
1	AA	602	A	C5-C6-N6	11.05	132.54	123.70
1	AA	687	A	C5-C6-N6	11.05	132.54	123.70
1	AA	919	A	C5-C6-N6	11.05	132.54	123.70
1	AA	1252	A	N7-C8-N9	-11.05	108.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1641	A	C5-C6-N6	11.05	132.54	123.70
26	BA	2266	A	C5-C6-N6	11.05	132.54	123.70
26	BA	2314	A	C5-C6-N6	11.05	132.54	123.70
26	BA	2358	A	C5-C6-N6	11.05	132.54	123.70
1	AA	1167	A	N7-C8-N9	-11.05	108.27	113.80
1	AA	238	A	C5-C6-N6	11.05	132.54	123.70
1	AA	1275	A	C5-C6-N6	11.05	132.54	123.70
1	AA	1360	A	C5-C6-N6	11.05	132.54	123.70
26	BA	980	A	C5-C6-N6	11.05	132.54	123.70
26	BA	693	A	C5-C6-N6	11.05	132.54	123.70
26	BA	936	A	C5-C6-N6	11.05	132.54	123.70
26	BA	1000	A	C5-C6-N6	11.05	132.54	123.70
26	BA	1885	A	C5-C6-N6	11.05	132.54	123.70
26	BA	1932	A	C5-C6-N6	11.05	132.54	123.70
1	AA	197	A	C5-C6-N6	11.04	132.53	123.70
26	BA	742	A	C5-C6-N6	11.04	132.53	123.70
26	BA	1551	A	C5-C6-N6	11.04	132.54	123.70
27	BB	15	A	C5-C6-N6	11.04	132.54	123.70
1	AA	152	A	C5-C6-N6	11.04	132.53	123.70
1	AA	649	A	C5-C6-N6	11.04	132.53	123.70
26	BA	2740	A	C5-C6-N6	11.04	132.53	123.70
26	BA	320	A	C5-C6-N6	11.04	132.53	123.70
26	BA	526	A	C5-C6-N6	11.04	132.53	123.70
26	BA	764	A	C5-C6-N6	11.04	132.53	123.70
26	BA	1654	A	C5-C6-N6	11.04	132.53	123.70
26	BA	1952	A	C5-C6-N6	11.04	132.53	123.70
26	BA	1819	A	C5-C6-N6	11.04	132.53	123.70
1	AA	16	A	C5-C6-N6	11.04	132.53	123.70
1	AA	1519	A	C5-C6-N6	11.04	132.53	123.70
26	BA	294	A	C5-C6-N6	11.04	132.53	123.70
26	BA	299	A	C5-C6-N6	11.04	132.53	123.70
26	BA	1342	A	C5-C6-N6	11.04	132.53	123.70
26	BA	2564	A	C5-C6-N6	11.04	132.53	123.70
26	BA	1919	A	C5-C6-N6	11.04	132.53	123.70
1	AA	1534	A	C5-C6-N6	11.04	132.53	123.70
26	BA	483	A	C5-C6-N6	11.04	132.53	123.70
1	AA	572	A	C5-C6-N6	11.03	132.53	123.70
1	AA	1152	A	N7-C8-N9	-11.03	108.28	113.80
26	BA	959	A	C5-C6-N6	11.03	132.53	123.70
26	BA	1853	A	C5-C6-N6	11.04	132.53	123.70
26	BA	2288	A	C5-C6-N6	11.03	132.53	123.70
26	BA	2327	A	N7-C8-N9	-11.04	108.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	76	A	C5-C6-N6	11.03	132.53	123.70
1	AA	320	A	C5-C6-N6	11.03	132.53	123.70
1	AA	574	A	C5-C6-N6	11.03	132.53	123.70
26	BA	1569	A	C5-C6-N6	11.03	132.53	123.70
26	BA	1664	A	N7-C8-N9	-11.03	108.28	113.80
26	BA	89	A	C5-C6-N6	11.03	132.53	123.70
26	BA	422	A	C5-C6-N6	11.03	132.53	123.70
26	BA	1039	A	C5-C6-N6	11.03	132.53	123.70
26	BA	1525	A	C5-C6-N6	11.03	132.53	123.70
26	BA	1616	A	C5-C6-N6	11.03	132.53	123.70
1	AA	718	A	C5-C6-N6	11.03	132.52	123.70
1	AA	1480	A	C5-C6-N6	11.03	132.52	123.70
24	AX	9	A	C5-C6-N6	11.03	132.52	123.70
1	AA	753	A	C5-C6-N6	11.03	132.52	123.70
26	BA	909	A	C5-C6-N6	11.03	132.52	123.70
26	BA	1854	A	C5-C6-N6	11.03	132.52	123.70
26	BA	2711	A	C5-C6-N6	11.03	132.52	123.70
26	BA	1189	A	C5-C6-N6	11.03	132.52	123.70
26	BA	1981	A	C5-C6-N6	11.03	132.52	123.70
1	AA	172	A	C5-C6-N6	11.03	132.52	123.70
1	AA	315	A	C5-C6-N6	11.03	132.52	123.70
1	AA	1246	A	C5-C6-N6	11.03	132.52	123.70
23	AW	73	A	C5-C6-N6	11.03	132.52	123.70
26	BA	1143	A	C5-C6-N6	11.03	132.52	123.70
26	BA	2741	A	C5-C6-N6	11.03	132.52	123.70
26	BA	429	A	C5-C6-N6	11.02	132.52	123.70
26	BA	1089	A	C5-C6-N6	11.02	132.52	123.70
26	BA	2753	A	C5-C6-N6	11.02	132.52	123.70
1	AA	465	A	C5-C6-N6	11.02	132.52	123.70
1	AA	1254	A	C5-C6-N6	11.02	132.52	123.70
26	BA	1876	A	N7-C8-N9	-11.02	108.29	113.80
26	BA	1913	A	C5-C6-N6	11.02	132.52	123.70
26	BA	2598	A	C5-C6-N6	11.02	132.52	123.70
26	BA	19	A	C5-C6-N6	11.02	132.52	123.70
26	BA	213	A	C5-C6-N6	11.02	132.52	123.70
26	BA	244	A	C5-C6-N6	11.02	132.52	123.70
26	BA	262	A	C5-C6-N6	11.02	132.52	123.70
26	BA	300	A	C5-C6-N6	11.02	132.52	123.70
26	BA	1009	A	C5-C6-N6	11.02	132.52	123.70
26	BA	2003	A	C5-C6-N6	11.02	132.52	123.70
26	BA	1786	A	C5-C6-N6	11.02	132.52	123.70
26	BA	2030	A	C5-C6-N6	11.02	132.52	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2346	A	C5-C6-N6	11.02	132.52	123.70
1	AA	412	A	C5-C6-N6	11.02	132.51	123.70
1	AA	1036	A	C5-C6-N6	11.02	132.51	123.70
1	AA	1250	A	C5-C6-N6	11.02	132.51	123.70
26	BA	384	A	N7-C8-N9	-11.02	108.29	113.80
26	BA	1275	A	C5-C6-N6	11.02	132.52	123.70
26	BA	528	A	C5-C6-N6	11.02	132.51	123.70
1	AA	728	A	C5-C6-N6	11.02	132.51	123.70
1	AA	777	A	C5-C6-N6	11.02	132.51	123.70
26	BA	478	A	C5-C6-N6	11.02	132.51	123.70
27	BB	94	A	C5-C6-N6	11.02	132.51	123.70
26	BA	988	A	C5-C6-N6	11.02	132.51	123.70
26	BA	1679	A	C5-C6-N6	11.02	132.51	123.70
26	BA	2657	A	C5-C6-N6	11.02	132.51	123.70
1	AA	655	A	C5-C6-N6	11.01	132.51	123.70
1	AA	759	A	C5-C6-N6	11.01	132.51	123.70
26	BA	632	A	N7-C8-N9	-11.01	108.29	113.80
26	BA	990	A	C5-C6-N6	11.01	132.51	123.70
26	BA	2278	A	C5-C6-N6	11.01	132.51	123.70
1	AA	780	A	C5-C6-N6	11.01	132.51	123.70
1	AA	1288	A	C5-C6-N6	11.01	132.51	123.70
1	AA	1531	A	C5-C6-N6	11.01	132.51	123.70
25	AY	21	A	C5-C6-N6	11.01	132.51	123.70
26	BA	310	A	C5-C6-N6	11.01	132.51	123.70
26	BA	1419	A	C5-C6-N6	11.01	132.51	123.70
26	BA	2577	A	C5-C6-N6	11.01	132.51	123.70
1	AA	78	A	C5-C6-N6	11.01	132.51	123.70
1	AA	949	A	C5-C6-N6	11.01	132.51	123.70
26	BA	603	A	C5-C6-N6	11.01	132.51	123.70
26	BA	735	A	C5-C6-N6	11.01	132.51	123.70
26	BA	947	A	C5-C6-N6	11.01	132.51	123.70
26	BA	1431	A	C5-C6-N6	11.01	132.51	123.70
26	BA	1890	A	C5-C6-N6	11.01	132.51	123.70
26	BA	1928	A	C5-C6-N6	11.01	132.51	123.70
26	BA	2135	A	C5-C6-N6	11.01	132.51	123.70
1	AA	51	A	C5-C6-N6	11.01	132.51	123.70
1	AA	695	A	C5-C6-N6	11.01	132.51	123.70
1	AA	958	A	C5-C6-N6	11.01	132.51	123.70
1	AA	1067	A	C5-C6-N6	11.01	132.51	123.70
1	AA	1493	A	C5-C6-N6	11.01	132.50	123.70
26	BA	1618	A	C5-C6-N6	11.01	132.51	123.70
26	BA	501	A	C5-C6-N6	11.01	132.50	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	899	A	C5-C6-N6	11.01	132.50	123.70
26	BA	1285	A	C5-C6-N6	11.01	132.50	123.70
26	BA	2173	A	C5-C6-N6	11.01	132.50	123.70
27	BB	104	A	C5-C6-N6	11.01	132.50	123.70
1	AA	189	A	C5-C6-N6	11.00	132.50	123.70
26	BA	2476	A	C5-C6-N6	11.00	132.50	123.70
27	BB	108	A	C5-C6-N6	11.00	132.50	123.70
1	AA	509	A	C5-C6-N6	11.00	132.50	123.70
26	BA	1142	A	C5-C6-N6	11.00	132.50	123.70
26	BA	1626	A	C5-C6-N6	11.00	132.50	123.70
26	BA	1877	A	C5-C6-N6	11.00	132.50	123.70
1	AA	196	A	C5-C6-N6	11.00	132.50	123.70
1	AA	493	A	C5-C6-N6	11.00	132.50	123.70
1	AA	792	A	C5-C6-N6	11.00	132.50	123.70
26	BA	160	A	C5-C6-N6	11.00	132.50	123.70
1	AA	1092	A	C5-C6-N6	11.00	132.50	123.70
26	BA	592	A	C5-C6-N6	11.00	132.50	123.70
26	BA	844	A	C5-C6-N6	11.00	132.50	123.70
26	BA	1927	A	C5-C6-N6	11.00	132.50	123.70
26	BA	2199	A	C5-C6-N6	11.00	132.50	123.70
26	BA	2503	A	C5-C6-N6	11.00	132.50	123.70
1	AA	1332	A	C5-C6-N6	11.00	132.50	123.70
26	BA	182	A	C5-C6-N6	11.00	132.50	123.70
26	BA	223	A	C5-C6-N6	11.00	132.50	123.70
26	BA	423	A	C5-C6-N6	11.00	132.50	123.70
26	BA	508	A	C5-C6-N6	11.00	132.50	123.70
26	BA	1307	A	C5-C6-N6	11.00	132.50	123.70
26	BA	2434	A	C5-C6-N6	11.00	132.50	123.70
26	BA	2598	A	N7-C8-N9	-11.00	108.30	113.80
26	BA	1439	A	C5-C6-N6	11.00	132.50	123.70
26	BA	1609	A	C5-C6-N6	11.00	132.50	123.70
26	BA	1809	A	C5-C6-N6	11.00	132.50	123.70
1	AA	246	A	C5-C6-N6	10.99	132.50	123.70
1	AA	338	A	C5-C6-N6	10.99	132.50	123.70
1	AA	996	A	C5-C6-N6	10.99	132.50	123.70
26	BA	28	A	C5-C6-N6	10.99	132.50	123.70
26	BA	788	A	C5-C6-N6	10.99	132.50	123.70
26	BA	1610	A	C5-C6-N6	10.99	132.50	123.70
26	BA	1689	A	C5-C6-N6	10.99	132.50	123.70
1	AA	3	A	C5-C6-N6	10.99	132.49	123.70
1	AA	72	A	C5-C6-N6	10.99	132.49	123.70
1	AA	441	A	C5-C6-N6	10.99	132.50	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	694	A	C5-C6-N6	10.99	132.49	123.70
1	AA	914	A	C5-C6-N6	10.99	132.49	123.70
26	BA	10	A	C5-C6-N6	10.99	132.50	123.70
26	BA	1084	A	C5-C6-N6	10.99	132.50	123.70
26	BA	265	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2270	A	C5-C6-N6	10.99	132.49	123.70
1	AA	535	A	C5-C6-N6	10.99	132.49	123.70
1	AA	794	A	C5-C6-N6	10.99	132.49	123.70
1	AA	815	A	C5-C6-N6	10.99	132.49	123.70
1	AA	1080	A	C5-C6-N6	10.99	132.49	123.70
26	BA	203	A	C5-C6-N6	10.99	132.49	123.70
26	BA	739	A	C5-C6-N6	10.99	132.49	123.70
26	BA	1032	A	C5-C6-N6	10.99	132.49	123.70
26	BA	1570	A	N7-C8-N9	-10.99	108.31	113.80
26	BA	2070	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2478	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2531	A	C5-C6-N6	10.99	132.49	123.70
1	AA	1191	A	C5-C6-N6	10.99	132.49	123.70
24	AX	58	A	C5-C6-N6	10.99	132.49	123.70
26	BA	219	A	C5-C6-N6	10.99	132.49	123.70
26	BA	345	A	C5-C6-N6	10.99	132.49	123.70
26	BA	563	A	C5-C6-N6	10.99	132.49	123.70
26	BA	670	A	C5-C6-N6	10.99	132.49	123.70
26	BA	1889	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2031	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2060	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2227	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2274	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2392	A	N7-C8-N9	-10.99	108.31	113.80
26	BA	94	A	C5-C6-N6	10.99	132.49	123.70
1	AA	59	A	C5-C6-N6	10.99	132.49	123.70
1	AA	298	A	C5-C6-N6	10.99	132.49	123.70
1	AA	1012	A	C5-C6-N6	10.99	132.49	123.70
23	AW	59	A	C5-C6-N6	10.99	132.49	123.70
26	BA	643	A	C5-C6-N6	10.99	132.49	123.70
26	BA	721	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2823	A	C5-C6-N6	10.99	132.49	123.70
26	BA	1598	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2117	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2212	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2448	A	C5-C6-N6	10.99	132.49	123.70
26	BA	2482	A	C5-C6-N6	10.99	132.49	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	155	A	C5-C6-N6	10.98	132.49	123.70
26	BA	616	A	C5-C6-N6	10.98	132.49	123.70
26	BA	1095	A	C5-C6-N6	10.98	132.49	123.70
26	BA	1420	A	C5-C6-N6	10.98	132.49	123.70
26	BA	1632	A	C5-C6-N6	10.98	132.49	123.70
1	AA	181	A	C5-C6-N6	10.98	132.49	123.70
26	BA	1265	A	C5-C6-N6	10.98	132.49	123.70
26	BA	1978	A	C5-C6-N6	10.98	132.49	123.70
26	BA	2126	A	C5-C6-N6	10.98	132.49	123.70
26	BA	2309	A	C5-C6-N6	10.98	132.49	123.70
1	AA	466	A	C5-C6-N6	10.98	132.49	123.70
1	AA	223	A	C5-C6-N6	10.98	132.48	123.70
1	AA	747	A	C5-C6-N6	10.98	132.49	123.70
1	AA	1430	A	C5-C6-N6	10.98	132.49	123.70
26	BA	497	A	C5-C6-N6	10.98	132.49	123.70
26	BA	613	A	C5-C6-N6	10.98	132.49	123.70
26	BA	877	A	C5-C6-N6	10.98	132.49	123.70
26	BA	911	A	C5-C6-N6	10.98	132.49	123.70
26	BA	1247	A	C5-C6-N6	10.98	132.49	123.70
26	BA	1701	A	C5-C6-N6	10.98	132.49	123.70
26	BA	892	A	C5-C6-N6	10.98	132.48	123.70
26	BA	2781	A	C5-C6-N6	10.98	132.49	123.70
1	AA	383	A	C5-C6-N6	10.98	132.48	123.70
1	AA	909	A	C5-C6-N6	10.98	132.48	123.70
26	BA	2328	A	N7-C8-N9	-10.98	108.31	113.80
1	AA	71	A	C5-C6-N6	10.98	132.48	123.70
1	AA	382	A	C5-C6-N6	10.98	132.48	123.70
22	AV	22	A	C5-C6-N6	10.98	132.48	123.70
26	BA	142	A	N7-C8-N9	-10.98	108.31	113.80
26	BA	1677	A	C5-C6-N6	10.98	132.48	123.70
26	BA	2058	A	C5-C6-N6	10.98	132.48	123.70
26	BA	2147	A	C5-C6-N6	10.98	132.48	123.70
1	AA	1503	A	C5-C6-N6	10.98	132.48	123.70
26	BA	344	A	C5-C6-N6	10.98	132.48	123.70
26	BA	368	A	C5-C6-N6	10.98	132.48	123.70
26	BA	532	A	N7-C8-N9	-10.98	108.31	113.80
26	BA	749	A	C5-C6-N6	10.98	132.48	123.70
26	BA	1069	A	C5-C6-N6	10.98	132.48	123.70
26	BA	1392	A	C5-C6-N6	10.98	132.48	123.70
26	BA	2051	A	C5-C6-N6	10.98	132.48	123.70
27	BB	101	A	C5-C6-N6	10.98	132.48	123.70
27	BB	115	A	C5-C6-N6	10.98	132.48	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1014	A	C5-C6-N6	10.97	132.48	123.70
1	AA	1179	A	C5-C6-N6	10.97	132.48	123.70
1	AA	1271	A	C5-C6-N6	10.97	132.48	123.70
22	AV	17	A	C5-C6-N6	10.97	132.48	123.70
26	BA	374	A	C5-C6-N6	10.97	132.48	123.70
26	BA	866	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1322	A	C5-C6-N6	10.97	132.48	123.70
1	AA	1163	A	C5-C6-N6	10.97	132.48	123.70
26	BA	127	A	C5-C6-N6	10.97	132.48	123.70
26	BA	507	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1020	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1098	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1336	A	C5-C6-N6	10.97	132.48	123.70
26	BA	2810	A	C5-C6-N6	10.97	132.48	123.70
1	AA	199	A	C5-C6-N6	10.97	132.48	123.70
24	AX	14	A	C5-C6-N6	10.97	132.48	123.70
26	BA	71	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1254	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1383	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1900	A	C5-C6-N6	10.97	132.48	123.70
26	BA	2183	A	C5-C6-N6	10.97	132.48	123.70
1	AA	60	A	C5-C6-N6	10.97	132.48	123.70
1	AA	768	A	C5-C6-N6	10.97	132.48	123.70
26	BA	602	A	C5-C6-N6	10.97	132.48	123.70
26	BA	927	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1579	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1650	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1580	A	C5-C6-N6	10.97	132.48	123.70
26	BA	1783	A	C5-C6-N6	10.97	132.47	123.70
26	BA	2809	A	C5-C6-N6	10.97	132.47	123.70
23	AW	51	A	C5-C6-N6	10.97	132.47	123.70
26	BA	792	A	C5-C6-N6	10.97	132.47	123.70
27	BB	119	A	C5-C6-N6	10.97	132.47	123.70
26	BA	900	A	C5-C6-N6	10.97	132.47	123.70
26	BA	1757	A	C5-C6-N6	10.97	132.47	123.70
26	BA	2682	A	C5-C6-N6	10.97	132.47	123.70
1	AA	1269	A	C5-C6-N6	10.97	132.47	123.70
24	AX	76	A	C5-C6-N6	10.97	132.47	123.70
26	BA	2042	A	C5-C6-N6	10.97	132.47	123.70
26	BA	2530	A	C5-C6-N6	10.97	132.47	123.70
26	BA	2850	A	C5-C6-N6	10.97	132.47	123.70
1	AA	279	A	C5-C6-N6	10.96	132.47	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	975	A	C5-C6-N6	10.96	132.47	123.70
23	AW	66	A	C5-C6-N6	10.96	132.47	123.70
26	BA	332	A	C5-C6-N6	10.96	132.47	123.70
26	BA	734	A	C5-C6-N6	10.96	132.47	123.70
26	BA	1046	A	C5-C6-N6	10.96	132.47	123.70
26	BA	1762	A	C5-C6-N6	10.96	132.47	123.70
1	AA	860	A	C5-C6-N6	10.96	132.47	123.70
1	AA	906	A	C5-C6-N6	10.96	132.47	123.70
1	AA	344	A	C5-C6-N6	10.96	132.47	123.70
1	AA	1196	A	C5-C6-N6	10.96	132.47	123.70
22	AV	21	A	C5-C6-N6	10.96	132.47	123.70
1	AA	366	A	C5-C6-N6	10.96	132.47	123.70
1	AA	1197	A	C5-C6-N6	10.96	132.47	123.70
1	AA	1518	A	C5-C6-N6	10.96	132.47	123.70
26	BA	443	A	C5-C6-N6	10.96	132.47	123.70
26	BA	1744	A	C5-C6-N6	10.96	132.47	123.70
26	BA	270	A	C5-C6-N6	10.96	132.47	123.70
26	BA	789	A	C5-C6-N6	10.96	132.47	123.70
26	BA	1847	A	C5-C6-N6	10.96	132.47	123.70
27	BB	58	A	C5-C6-N6	10.96	132.47	123.70
26	BA	2037	A	C5-C6-N6	10.96	132.47	123.70
26	BA	2738	A	C5-C6-N6	10.96	132.47	123.70
1	AA	143	A	C5-C6-N6	10.96	132.47	123.70
1	AA	459	A	C5-C6-N6	10.96	132.47	123.70
26	BA	391	A	C5-C6-N6	10.96	132.47	123.70
26	BA	432	A	C5-C6-N6	10.96	132.47	123.70
26	BA	637	A	C5-C6-N6	10.96	132.47	123.70
26	BA	1021	A	C5-C6-N6	10.96	132.47	123.70
1	AA	630	A	C5-C6-N6	10.96	132.47	123.70
1	AA	1111	A	C5-C6-N6	10.96	132.47	123.70
26	BA	309	A	C5-C6-N6	10.96	132.47	123.70
26	BA	1021	A	N7-C8-N9	-10.96	108.32	113.80
26	BA	1808	A	C5-C6-N6	10.96	132.47	123.70
26	BA	1998	A	C5-C6-N6	10.96	132.47	123.70
1	AA	282	A	C5-C6-N6	10.96	132.47	123.70
1	AA	520	A	C5-C6-N6	10.96	132.46	123.70
1	AA	696	A	C5-C6-N6	10.96	132.46	123.70
26	BA	626	A	C5-C6-N6	10.96	132.47	123.70
26	BA	1133	A	C5-C6-N6	10.96	132.46	123.70
26	BA	1272	A	C5-C6-N6	10.96	132.47	123.70
26	BA	1700	A	C5-C6-N6	10.96	132.47	123.70
26	BA	2820	A	C5-C6-N6	10.96	132.47	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	845	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1146	A	C5-C6-N6	10.95	132.46	123.70
25	AY	73	A	C5-C6-N6	10.95	132.46	123.70
26	BA	125	A	C5-C6-N6	10.96	132.46	123.70
26	BA	2679	A	C5-C6-N6	10.96	132.46	123.70
26	BA	2883	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2886	A	C5-C6-N6	10.95	132.46	123.70
1	AA	19	A	C5-C6-N6	10.95	132.46	123.70
1	AA	50	A	C5-C6-N6	10.95	132.46	123.70
1	AA	595	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1016	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1042	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1287	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1408	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1502	A	C5-C6-N6	10.95	132.46	123.70
24	AX	21	A	C5-C6-N6	10.95	132.46	123.70
26	BA	632	A	C5-C6-N6	10.95	132.46	123.70
26	BA	1010	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2311	A	C5-C6-N6	10.95	132.46	123.70
26	BA	13	A	C5-C6-N6	10.95	132.46	123.70
26	BA	1054	A	C5-C6-N6	10.95	132.46	123.70
26	BA	1085	A	C5-C6-N6	10.95	132.46	123.70
26	BA	1509	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2281	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2542	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2727	A	C5-C6-N6	10.95	132.46	123.70
27	BB	73	A	C5-C6-N6	10.95	132.46	123.70
1	AA	77	A	C5-C6-N6	10.95	132.46	123.70
1	AA	547	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1394	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1398	A	C5-C6-N6	10.95	132.46	123.70
26	BA	218	A	C5-C6-N6	10.95	132.46	123.70
26	BA	627	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2432	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2873	A	C5-C6-N6	10.95	132.46	123.70
26	BA	515	A	C5-C6-N6	10.95	132.46	123.70
26	BA	960	A	N7-C8-N9	-10.95	108.33	113.80
26	BA	1175	A	C5-C6-N6	10.95	132.46	123.70
26	BA	1287	A	C5-C6-N6	10.95	132.46	123.70
26	BA	1717	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2733	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2814	A	C5-C6-N6	10.95	132.46	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	767	A	C5-C6-N6	10.95	132.46	123.70
1	AA	787	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1117	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1285	A	C5-C6-N6	10.95	132.46	123.70
26	BA	1918	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2758	A	C5-C6-N6	10.95	132.46	123.70
1	AA	607	A	C5-C6-N6	10.94	132.46	123.70
1	AA	900	A	C5-C6-N6	10.94	132.46	123.70
1	AA	913	A	C5-C6-N6	10.94	132.46	123.70
1	AA	977	A	C5-C6-N6	10.94	132.46	123.70
1	AA	1093	A	C5-C6-N6	10.94	132.46	123.70
1	AA	1431	A	C5-C6-N6	10.95	132.46	123.70
26	BA	14	A	C5-C6-N6	10.95	132.46	123.70
1	AA	1500	A	C5-C6-N6	10.94	132.46	123.70
26	BA	226	A	C5-C6-N6	10.95	132.46	123.70
26	BA	322	A	C5-C6-N6	10.95	132.46	123.70
26	BA	1552	A	C5-C6-N6	10.94	132.46	123.70
26	BA	2062	A	C5-C6-N6	10.94	132.46	123.70
26	BA	2378	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2602	A	C5-C6-N6	10.95	132.46	123.70
26	BA	2900	A	C5-C6-N6	10.95	132.46	123.70
27	BB	53	A	C5-C6-N6	10.94	132.46	123.70
1	AA	892	A	C5-C6-N6	10.94	132.45	123.70
1	AA	1110	A	C5-C6-N6	10.94	132.45	123.70
1	AA	1239	A	C5-C6-N6	10.94	132.45	123.70
26	BA	1214	A	C5-C6-N6	10.94	132.46	123.70
26	BA	216	A	C5-C6-N6	10.94	132.45	123.70
26	BA	502	A	C5-C6-N6	10.94	132.45	123.70
26	BA	2750	A	C5-C6-N6	10.94	132.46	123.70
26	BA	547	A	C5-C6-N6	10.94	132.45	123.70
26	BA	655	A	C5-C6-N6	10.94	132.45	123.70
26	BA	715	A	C5-C6-N6	10.94	132.45	123.70
26	BA	1544	A	C5-C6-N6	10.94	132.45	123.70
26	BA	2813	A	C5-C6-N6	10.94	132.45	123.70
26	BA	2872	A	C5-C6-N6	10.94	132.45	123.70
26	BA	348	A	C5-C6-N6	10.94	132.45	123.70
26	BA	477	A	C5-C6-N6	10.94	132.45	123.70
26	BA	878	A	C5-C6-N6	10.94	132.45	123.70
26	BA	1230	A	C5-C6-N6	10.94	132.45	123.70
26	BA	1912	A	C5-C6-N6	10.94	132.45	123.70
26	BA	2411	A	C5-C6-N6	10.94	132.45	123.70
1	AA	704	A	C5-C6-N6	10.94	132.45	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1499	A	C5-C6-N6	10.94	132.45	123.70
1	AA	468	A	C5-C6-N6	10.94	132.45	123.70
1	AA	559	A	C5-C6-N6	10.94	132.45	123.70
1	AA	673	A	C5-C6-N6	10.94	132.45	123.70
1	AA	807	A	C5-C6-N6	10.94	132.45	123.70
26	BA	103	A	C5-C6-N6	10.94	132.45	123.70
26	BA	654	A	C5-C6-N6	10.94	132.45	123.70
26	BA	504	A	C5-C6-N6	10.94	132.45	123.70
26	BA	984	A	C5-C6-N6	10.94	132.45	123.70
26	BA	1048	A	C5-C6-N6	10.94	132.45	123.70
26	BA	1067	A	C5-C6-N6	10.94	132.45	123.70
26	BA	1373	A	C5-C6-N6	10.94	132.45	123.70
26	BA	1433	A	C5-C6-N6	10.94	132.45	123.70
26	BA	1780	A	C5-C6-N6	10.94	132.45	123.70
26	BA	1872	A	C5-C6-N6	10.94	132.45	123.70
1	AA	65	A	C5-C6-N6	10.93	132.45	123.70
1	AA	563	A	N7-C8-N9	-10.93	108.33	113.80
1	AA	663	A	C5-C6-N6	10.93	132.45	123.70
1	AA	968	A	C5-C6-N6	10.93	132.45	123.70
23	AW	21	A	C5-C6-N6	10.93	132.44	123.70
23	AW	31	A	C5-C6-N6	10.93	132.45	123.70
23	AW	38	A	C5-C6-N6	10.93	132.45	123.70
26	BA	479	A	C5-C6-N6	10.93	132.45	123.70
26	BA	1129	A	C5-C6-N6	10.93	132.45	123.70
26	BA	1495	A	C5-C6-N6	10.93	132.45	123.70
26	BA	2198	A	C5-C6-N6	10.93	132.45	123.70
26	BA	2268	A	C5-C6-N6	10.93	132.45	123.70
26	BA	2377	A	C5-C6-N6	10.93	132.45	123.70
26	BA	2654	A	C5-C6-N6	10.93	132.44	123.70
1	AA	120	A	C5-C6-N6	10.93	132.44	123.70
1	AA	642	A	C5-C6-N6	10.93	132.44	123.70
1	AA	790	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1050	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1583	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1678	A	C5-C6-N6	10.93	132.44	123.70
26	BA	2119	A	C5-C6-N6	10.93	132.44	123.70
1	AA	250	A	C5-C6-N6	10.93	132.44	123.70
1	AA	819	A	C5-C6-N6	10.93	132.44	123.70
1	AA	946	A	C5-C6-N6	10.93	132.44	123.70
1	AA	1447	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1354	A	C5-C6-N6	10.93	132.44	123.70
25	AY	26	A	C5-C6-N6	10.93	132.44	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	83	A	C5-C6-N6	10.93	132.44	123.70
26	BA	167	A	C5-C6-N6	10.93	132.44	123.70
26	BA	761	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1111	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1802	A	C5-C6-N6	10.93	132.44	123.70
26	BA	2893	A	C5-C6-N6	10.93	132.44	123.70
1	AA	363	A	C5-C6-N6	10.93	132.44	123.70
1	AA	1257	A	C5-C6-N6	10.93	132.44	123.70
26	BA	466	A	N7-C8-N9	-10.93	108.34	113.80
26	BA	1366	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1899	A	N7-C8-N9	-10.93	108.34	113.80
1	AA	1046	A	C5-C6-N6	10.93	132.44	123.70
1	AA	1188	A	C5-C6-N6	10.93	132.44	123.70
1	AA	1256	A	C5-C6-N6	10.93	132.44	123.70
1	AA	1434	A	C5-C6-N6	10.93	132.44	123.70
25	AY	35	A	C5-C6-N6	10.93	132.44	123.70
26	BA	221	A	C5-C6-N6	10.93	132.44	123.70
26	BA	384	A	C5-C6-N6	10.93	132.44	123.70
26	BA	590	A	C5-C6-N6	10.93	132.44	123.70
26	BA	945	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1080	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1321	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1367	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1635	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1759	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1815	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1936	A	C5-C6-N6	10.93	132.44	123.70
26	BA	1966	A	C5-C6-N6	10.93	132.44	123.70
26	BA	2267	A	N7-C8-N9	-10.93	108.34	113.80
26	BA	2835	A	C5-C6-N6	10.93	132.44	123.70
1	AA	600	A	C5-C6-N6	10.92	132.44	123.70
1	AA	629	A	C5-C6-N6	10.92	132.44	123.70
26	BA	2726	A	C5-C6-N6	10.92	132.44	123.70
1	AA	28	A	C5-C6-N6	10.92	132.44	123.70
1	AA	119	A	C5-C6-N6	10.92	132.44	123.70
1	AA	130	A	C5-C6-N6	10.92	132.44	123.70
1	AA	729	A	C5-C6-N6	10.92	132.44	123.70
1	AA	1319	A	C5-C6-N6	10.92	132.44	123.70
26	BA	73	A	C5-C6-N6	10.92	132.44	123.70
26	BA	161	A	C5-C6-N6	10.92	132.44	123.70
26	BA	324	A	C5-C6-N6	10.92	132.44	123.70
26	BA	609	A	C5-C6-N6	10.92	132.44	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1096	A	C5-C6-N6	10.92	132.44	123.70
26	BA	1302	A	C5-C6-N6	10.92	132.44	123.70
26	BA	1384	A	C5-C6-N6	10.92	132.44	123.70
26	BA	1705	A	C5-C6-N6	10.92	132.44	123.70
26	BA	2821	A	C5-C6-N6	10.92	132.44	123.70
27	BB	99	A	C5-C6-N6	10.92	132.44	123.70
27	BB	109	A	C5-C6-N6	10.92	132.44	123.70
1	AA	288	A	C5-C6-N6	10.92	132.44	123.70
26	BA	2534	A	C5-C6-N6	10.92	132.44	123.70
1	AA	596	A	C5-C6-N6	10.92	132.44	123.70
1	AA	1492	A	C5-C6-N6	10.92	132.44	123.70
25	AY	14	A	C5-C6-N6	10.92	132.44	123.70
25	AY	41	A	C5-C6-N6	10.92	132.44	123.70
26	BA	149	A	C5-C6-N6	10.92	132.44	123.70
26	BA	195	A	C5-C6-N6	10.92	132.44	123.70
26	BA	781	A	C5-C6-N6	10.92	132.44	123.70
26	BA	428	A	C5-C6-N6	10.92	132.44	123.70
26	BA	1365	A	C5-C6-N6	10.92	132.44	123.70
26	BA	1672	A	C5-C6-N6	10.92	132.44	123.70
1	AA	236	A	C5-C6-N6	10.92	132.44	123.70
1	AA	831	A	C5-C6-N6	10.92	132.43	123.70
1	AA	1169	A	C5-C6-N6	10.92	132.43	123.70
26	BA	412	A	C5-C6-N6	10.92	132.43	123.70
26	BA	2317	A	C5-C6-N6	10.92	132.43	123.70
26	BA	2851	A	C5-C6-N6	10.92	132.44	123.70
1	AA	1377	A	C5-C6-N6	10.92	132.43	123.70
1	AA	1433	A	C5-C6-N6	10.92	132.43	123.70
1	AA	1441	A	C5-C6-N6	10.92	132.43	123.70
22	AV	15	A	C5-C6-N6	10.92	132.43	123.70
26	BA	2660	A	C5-C6-N6	10.92	132.43	123.70
1	AA	7	A	C5-C6-N6	10.91	132.43	123.70
1	AA	937	A	C5-C6-N6	10.91	132.43	123.70
23	AW	58	A	C5-C6-N6	10.91	132.43	123.70
26	BA	608	A	C5-C6-N6	10.91	132.43	123.70
26	BA	675	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1134	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1301	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1597	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1640	A	C5-C6-N6	10.91	132.43	123.70
26	BA	2327	A	C5-C6-N6	10.91	132.43	123.70
26	BA	2705	A	C5-C6-N6	10.91	132.43	123.70
26	BA	2721	A	C5-C6-N6	10.91	132.43	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	262	A	C5-C6-N6	10.91	132.43	123.70
1	AA	461	A	C5-C6-N6	10.91	132.43	123.70
1	AA	579	A	C5-C6-N6	10.91	132.43	123.70
1	AA	974	A	C5-C6-N6	10.91	132.43	123.70
26	BA	197	A	C5-C6-N6	10.91	132.43	123.70
26	BA	311	A	C5-C6-N6	10.91	132.43	123.70
26	BA	782	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1403	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1848	A	C5-C6-N6	10.91	132.43	123.70
26	BA	2376	A	C5-C6-N6	10.91	132.43	123.70
1	AA	116	A	C5-C6-N6	10.91	132.43	123.70
1	AA	160	A	C5-C6-N6	10.91	132.43	123.70
24	AX	26	A	C5-C6-N6	10.91	132.43	123.70
26	BA	342	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1205	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1274	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1477	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1596	A	C5-C6-N6	10.91	132.43	123.70
26	BA	1690	A	C5-C6-N6	10.91	132.43	123.70
25	AY	38	A	C5-C6-N6	10.91	132.43	123.70
1	AA	8	A	C5-C6-N6	10.91	132.43	123.70
1	AA	712	A	C5-C6-N6	10.91	132.43	123.70
26	BA	2433	A	C5-C6-N6	10.91	132.43	123.70
26	BA	2614	A	C5-C6-N6	10.91	132.43	123.70
1	AA	1213	A	C5-C6-N6	10.91	132.42	123.70
1	AA	1274	A	C5-C6-N6	10.91	132.43	123.70
26	BA	340	A	C5-C6-N6	10.91	132.43	123.70
26	BA	541	A	C5-C6-N6	10.91	132.42	123.70
26	BA	1264	A	C5-C6-N6	10.91	132.43	123.70
26	BA	2826	A	C5-C6-N6	10.91	132.43	123.70
1	AA	364	A	C5-C6-N6	10.90	132.42	123.70
1	AA	448	A	C5-C6-N6	10.90	132.42	123.70
1	AA	1145	A	C5-C6-N6	10.90	132.42	123.70
26	BA	804	A	C5-C6-N6	10.90	132.42	123.70
26	BA	1916	A	C5-C6-N6	10.90	132.42	123.70
1	AA	702	A	C5-C6-N6	10.90	132.42	123.70
1	AA	715	A	C5-C6-N6	10.90	132.42	123.70
1	AA	1176	A	C5-C6-N6	10.90	132.42	123.70
1	AA	1216	A	C5-C6-N6	10.90	132.42	123.70
26	BA	101	A	C5-C6-N6	10.90	132.42	123.70
26	BA	793	A	C5-C6-N6	10.90	132.42	123.70
26	BA	979	A	C5-C6-N6	10.90	132.42	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1528	A	C5-C6-N6	10.90	132.42	123.70
26	BA	2170	A	C5-C6-N6	10.90	132.42	123.70
26	BA	2860	A	C5-C6-N6	10.90	132.42	123.70
27	BB	39	A	C5-C6-N6	10.90	132.42	123.70
1	AA	306	A	C5-C6-N6	10.90	132.42	123.70
1	AA	325	A	C5-C6-N6	10.90	132.42	123.70
26	BA	492	A	C5-C6-N6	10.90	132.42	123.70
1	AA	1019	A	C5-C6-N6	10.90	132.42	123.70
1	AA	1180	A	C5-C6-N6	10.90	132.42	123.70
26	BA	222	A	C5-C6-N6	10.90	132.42	123.70
26	BA	1127	A	C5-C6-N6	10.90	132.42	123.70
26	BA	1508	A	C5-C6-N6	10.90	132.42	123.70
26	BA	1669	A	N3-C4-C5	-10.90	119.17	126.80
26	BA	1773	A	C5-C6-N6	10.90	132.42	123.70
26	BA	1871	A	C5-C6-N6	10.90	132.42	123.70
1	AA	487	A	C5-C6-N6	10.90	132.42	123.70
1	AA	496	A	C5-C6-N6	10.90	132.42	123.70
1	AA	781	A	C5-C6-N6	10.90	132.42	123.70
1	AA	1130	A	C5-C6-N6	10.90	132.42	123.70
26	BA	49	A	C5-C6-N6	10.90	132.42	123.70
22	AV	20	A	C5-C6-N6	10.90	132.42	123.70
26	BA	251	A	N7-C8-N9	-10.90	108.35	113.80
26	BA	666	A	C5-C6-N6	10.90	132.42	123.70
26	BA	1027	A	C5-C6-N6	10.90	132.42	123.70
26	BA	2163	A	C5-C6-N6	10.90	132.42	123.70
1	AA	109	A	C5-C6-N6	10.89	132.42	123.70
1	AA	635	A	C5-C6-N6	10.89	132.41	123.70
1	AA	676	A	C5-C6-N6	10.89	132.42	123.70
1	AA	872	A	N7-C8-N9	-10.89	108.35	113.80
26	BA	144	A	C5-C6-N6	10.89	132.41	123.70
26	BA	181	A	C5-C6-N6	10.89	132.42	123.70
26	BA	896	A	C5-C6-N6	10.89	132.42	123.70
26	BA	362	A	C5-C6-N6	10.89	132.41	123.70
26	BA	716	A	C5-C6-N6	10.89	132.41	123.70
26	BA	1698	A	C5-C6-N6	10.89	132.41	123.70
26	BA	2425	A	C5-C6-N6	10.89	132.41	123.70
26	BA	2426	A	C5-C6-N6	10.89	132.41	123.70
1	AA	546	A	N7-C8-N9	-10.89	108.35	113.80
23	AW	14	A	C5-C6-N6	10.89	132.41	123.70
24	AX	41	A	C5-C6-N6	10.89	132.41	123.70
26	BA	727	A	C5-C6-N6	10.89	132.41	123.70
26	BA	752	A	C5-C6-N6	10.89	132.41	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1156	A	C5-C6-N6	10.89	132.41	123.70
26	BA	1393	A	C5-C6-N6	10.89	132.41	123.70
26	BA	1434	A	C5-C6-N6	10.89	132.41	123.70
26	BA	2497	A	C5-C6-N6	10.89	132.41	123.70
1	AA	560	A	C5-C6-N6	10.89	132.41	123.70
1	AA	161	A	C5-C6-N6	10.89	132.41	123.70
1	AA	321	A	C5-C6-N6	10.89	132.41	123.70
1	AA	784	A	C5-C6-N6	10.89	132.41	123.70
1	AA	1251	A	C5-C6-N6	10.89	132.41	123.70
26	BA	172	A	C5-C6-N6	10.89	132.41	123.70
26	BA	928	A	C5-C6-N6	10.89	132.41	123.70
26	BA	1453	A	C5-C6-N6	10.89	132.41	123.70
26	BA	1746	A	C5-C6-N6	10.89	132.41	123.70
26	BA	2352	A	C5-C6-N6	10.89	132.41	123.70
26	BA	2792	A	C5-C6-N6	10.89	132.41	123.70
27	BB	57	A	C5-C6-N6	10.89	132.41	123.70
1	AA	228	A	C5-C6-N6	10.89	132.41	123.70
1	AA	1101	A	C5-C6-N6	10.88	132.41	123.70
1	AA	1261	A	C5-C6-N6	10.88	132.41	123.70
22	AV	19	A	C5-C6-N6	10.88	132.41	123.70
26	BA	126	A	C5-C6-N6	10.88	132.41	123.70
26	BA	1535	A	C5-C6-N6	10.89	132.41	123.70
26	BA	2059	A	C5-C6-N6	10.89	132.41	123.70
26	BA	472	A	C5-C6-N6	10.88	132.41	123.70
1	AA	609	A	C5-C6-N6	10.88	132.41	123.70
26	BA	2211	A	C5-C6-N6	10.88	132.41	123.70
1	AA	675	A	C5-C6-N6	10.88	132.40	123.70
26	BA	1470	A	C5-C6-N6	10.88	132.40	123.70
26	BA	2518	A	C5-C6-N6	10.88	132.41	123.70
1	AA	1362	A	C5-C6-N6	10.88	132.40	123.70
26	BA	2052	A	C5-C6-N6	10.88	132.40	123.70
1	AA	415	A	C5-C6-N6	10.88	132.40	123.70
1	AA	1446	A	C5-C6-N6	10.88	132.40	123.70
26	BA	718	A	C5-C6-N6	10.88	132.40	123.70
26	BA	751	A	C5-C6-N6	10.88	132.40	123.70
26	BA	1008	A	C5-C6-N6	10.88	132.40	123.70
26	BA	2406	A	C5-C6-N6	10.88	132.40	123.70
26	BA	2587	A	C5-C6-N6	10.88	132.40	123.70
26	BA	2887	A	C5-C6-N6	10.88	132.40	123.70
27	BB	46	A	C5-C6-N6	10.88	132.40	123.70
1	AA	510	A	C5-C6-N6	10.88	132.40	123.70
1	AA	964	A	C5-C6-N6	10.88	132.40	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1346	A	C5-C6-N6	10.88	132.40	123.70
26	BA	1088	A	C5-C6-N6	10.88	132.40	123.70
26	BA	482	A	C5-C6-N6	10.87	132.40	123.70
26	BA	2662	A	N7-C8-N9	-10.88	108.36	113.80
1	AA	116	A	N7-C8-N9	-10.87	108.36	113.80
1	AA	274	A	C5-C6-N6	10.87	132.40	123.70
1	AA	532	A	C5-C6-N6	10.87	132.40	123.70
26	BA	453	A	C5-C6-N6	10.87	132.40	123.70
26	BA	820	A	C5-C6-N6	10.87	132.40	123.70
26	BA	1126	A	C5-C6-N6	10.87	132.40	123.70
26	BA	2468	A	C5-C6-N6	10.87	132.40	123.70
26	BA	1028	A	C5-C6-N6	10.87	132.40	123.70
1	AA	2	A	C5-C6-N6	10.87	132.39	123.70
26	BA	505	A	C5-C6-N6	10.87	132.39	123.70
1	AA	81	A	C5-C6-N6	10.87	132.39	123.70
1	AA	1299	A	C5-C6-N6	10.87	132.39	123.70
26	BA	404	A	C5-C6-N6	10.86	132.39	123.70
26	BA	1226	A	C5-C6-N6	10.87	132.39	123.70
26	BA	1284	A	C5-C6-N6	10.87	132.39	123.70
26	BA	1789	A	C5-C6-N6	10.87	132.39	123.70
1	AA	1081	A	C5-C6-N6	10.86	132.39	123.70
26	BA	91	A	C5-C6-N6	10.86	132.39	123.70
26	BA	196	A	C5-C6-N6	10.86	132.39	123.70
26	BA	272	A	C5-C6-N6	10.86	132.39	123.70
26	BA	279	A	C5-C6-N6	10.86	132.39	123.70
26	BA	699	A	C5-C6-N6	10.86	132.39	123.70
26	BA	943	A	C5-C6-N6	10.86	132.39	123.70
26	BA	1103	A	C5-C6-N6	10.86	132.39	123.70
1	AA	414	A	C5-C6-N6	10.86	132.39	123.70
1	AA	1004	A	C5-C6-N6	10.86	132.39	123.70
1	AA	1105	A	C5-C6-N6	10.86	132.39	123.70
25	AY	58	A	C5-C6-N6	10.86	132.39	123.70
26	BA	920	A	C5-C6-N6	10.86	132.39	123.70
26	BA	2412	A	C5-C6-N6	10.86	132.39	123.70
26	BA	975	A	C5-C6-N6	10.86	132.39	123.70
26	BA	1505	A	C5-C6-N6	10.86	132.39	123.70
26	BA	2439	A	C5-C6-N6	10.86	132.39	123.70
1	AA	389	A	C5-C6-N6	10.86	132.38	123.70
26	BA	21	A	C5-C6-N6	10.86	132.38	123.70
26	BA	118	A	C5-C6-N6	10.86	132.38	123.70
26	BA	575	A	C5-C6-N6	10.86	132.38	123.70
26	BA	1858	A	C5-C6-N6	10.86	132.38	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1167	A	C5-C6-N6	10.85	132.38	123.70
1	AA	1456	A	C5-C6-N6	10.85	132.38	123.70
26	BA	6	A	C5-C6-N6	10.85	132.38	123.70
26	BA	1522	A	C5-C6-N6	10.85	132.38	123.70
26	BA	2700	A	C5-C6-N6	10.85	132.38	123.70
26	BA	1253	A	C5-C6-N6	10.85	132.38	123.70
26	BA	1359	A	C5-C6-N6	10.85	132.38	123.70
26	BA	2749	A	C5-C6-N6	10.85	132.38	123.70
1	AA	205	A	C5-C6-N6	10.85	132.38	123.70
26	BA	382	A	C5-C6-N6	10.85	132.38	123.70
26	BA	631	A	C5-C6-N6	10.85	132.38	123.70
26	BA	941	A	C5-C6-N6	10.85	132.38	123.70
26	BA	2430	A	N3-C4-C5	-10.85	119.20	126.80
26	BA	2670	A	C5-C6-N6	10.85	132.38	123.70
26	BA	2635	A	C5-C6-N6	10.85	132.38	123.70
26	BA	278	A	C5-C6-N6	10.85	132.38	123.70
26	BA	1711	A	C5-C6-N6	10.85	132.38	123.70
26	BA	2297	A	N7-C8-N9	-10.85	108.38	113.80
26	BA	2634	A	C5-C6-N6	10.85	132.38	123.70
1	AA	373	A	C5-C6-N6	10.84	132.38	123.70
26	BA	1722	A	C5-C6-N6	10.84	132.38	123.70
26	BA	199	A	C5-C6-N6	10.84	132.37	123.70
26	BA	730	A	C5-C6-N6	10.84	132.37	123.70
26	BA	1327	A	C5-C6-N6	10.84	132.37	123.70
26	BA	2333	A	C5-C6-N6	10.84	132.37	123.70
26	BA	2879	A	C5-C6-N6	10.84	132.37	123.70
1	AA	918	A	C5-C6-N6	10.84	132.37	123.70
1	AA	1306	A	C5-C6-N6	10.84	132.37	123.70
25	AY	23	A	C5-C6-N6	10.84	132.37	123.70
26	BA	1328	A	C5-C6-N6	10.84	132.37	123.70
26	BA	44	A	C5-C6-N6	10.84	132.37	123.70
26	BA	1151	A	C5-C6-N6	10.84	132.37	123.70
26	BA	1490	A	C5-C6-N6	10.84	132.37	123.70
26	BA	821	A	C5-C6-N6	10.84	132.37	123.70
26	BA	833	A	C5-C6-N6	10.84	132.37	123.70
26	BA	1269	A	C5-C6-N6	10.84	132.37	123.70
26	BA	2369	A	C5-C6-N6	10.84	132.37	123.70
1	AA	1252	A	C5-C6-N6	10.83	132.37	123.70
1	AA	1396	A	C5-C6-N6	10.83	132.37	123.70
26	BA	996	A	C5-C6-N6	10.83	132.37	123.70
26	BA	1754	A	C5-C6-N6	10.83	132.37	123.70
26	BA	2097	A	C5-C6-N6	10.83	132.37	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	621	A	C5-C6-N6	10.83	132.36	123.70
1	AA	983	A	C5-C6-N6	10.83	132.36	123.70
1	AA	994	A	C5-C6-N6	10.83	132.36	123.70
26	BA	146	A	C5-C6-N6	10.83	132.36	123.70
26	BA	2020	A	C5-C6-N6	10.83	132.36	123.70
26	BA	1735	A	C5-C6-N6	10.83	132.36	123.70
1	AA	174	A	C5-C6-N6	10.83	132.36	123.70
26	BA	722	A	C5-C6-N6	10.83	132.36	123.70
1	AA	397	A	N3-C4-C5	-10.82	119.22	126.80
26	BA	556	A	C5-C6-N6	10.82	132.36	123.70
26	BA	2340	A	C5-C6-N6	10.82	132.36	123.70
26	BA	401	A	C5-C6-N6	10.82	132.36	123.70
26	BA	2287	A	N7-C8-N9	-10.82	108.39	113.80
26	BA	5	A	C5-C6-N6	10.82	132.36	123.70
26	BA	972	A	C5-C6-N6	10.82	132.36	123.70
1	AA	1375	A	C5-C6-N6	10.82	132.35	123.70
26	BA	233	A	C5-C6-N6	10.82	132.36	123.70
26	BA	1713	A	C5-C6-N6	10.82	132.35	123.70
24	AX	3	A	C5-C6-N6	10.81	132.35	123.70
1	AA	716	A	C5-C6-N6	10.81	132.35	123.70
1	AA	1280	A	C5-C6-N6	10.81	132.35	123.70
1	AA	167	A	C5-C6-N6	10.81	132.35	123.70
1	AA	1236	A	C5-C6-N6	10.81	132.35	123.70
1	AA	553	A	C5-C6-N6	10.81	132.35	123.70
25	AY	69	A	C5-C6-N6	10.81	132.35	123.70
26	BA	614	A	C5-C6-N6	10.81	132.35	123.70
1	AA	397	A	N7-C8-N9	-10.80	108.40	113.80
1	AA	1035	A	C5-C6-N6	10.80	132.34	123.70
26	BA	2095	A	C5-C6-N6	10.80	132.34	123.70
26	BA	2328	A	C5-C6-N6	10.80	132.34	123.70
1	AA	1201	A	C5-C6-N6	10.80	132.34	123.70
26	BA	1787	A	C5-C6-N6	10.80	132.34	123.70
26	BA	439	A	C5-C6-N6	10.80	132.34	123.70
26	BA	1655	A	C5-C6-N6	10.80	132.34	123.70
26	BA	2158	A	C5-C6-N6	10.80	132.34	123.70
26	BA	2665	A	C5-C6-N6	10.80	132.34	123.70
26	BA	1739	A	C5-C6-N6	10.80	132.34	123.70
26	BA	522	A	C5-C6-N6	10.80	132.34	123.70
26	BA	1144	A	C5-C6-N6	10.80	132.34	123.70
26	BA	1469	A	C5-C6-N6	10.80	132.34	123.70
1	AA	303	A	C5-C6-N6	10.79	132.34	123.70
26	BA	352	A	C5-C6-N6	10.79	132.34	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	706	A	C5-C6-N6	10.79	132.34	123.70
26	BA	2114	A	C5-C6-N6	10.79	132.34	123.70
26	BA	2541	A	C5-C6-N6	10.79	132.34	123.70
1	AA	907	A	C5-C6-N6	10.79	132.34	123.70
26	BA	1977	A	C5-C6-N6	10.79	132.33	123.70
1	AA	523	A	C5-C6-N6	10.79	132.33	123.70
26	BA	95	A	C5-C6-N6	10.79	132.33	123.70
26	BA	1591	A	C5-C6-N6	10.79	132.33	123.70
26	BA	2366	A	C5-C6-N6	10.79	132.33	123.70
26	BA	227	A	C5-C6-N6	10.79	132.33	123.70
26	BA	282	A	C5-C6-N6	10.79	132.33	123.70
26	BA	1801	A	C5-C6-N6	10.79	132.33	123.70
1	AA	1465	A	C5-C6-N6	10.79	132.33	123.70
26	BA	256	A	C5-C6-N6	10.79	132.33	123.70
26	BA	1665	A	C5-C6-N6	10.79	132.33	123.70
26	BA	2082	A	C5-C6-N6	10.78	132.33	123.70
26	BA	251	A	C5-C6-N6	10.78	132.33	123.70
1	AA	353	A	C5-C6-N6	10.78	132.32	123.70
26	BA	402	A	C5-C6-N6	10.78	132.32	123.70
1	AA	1171	A	C5-C6-N6	10.78	132.32	123.70
26	BA	1566	A	C5-C6-N6	10.78	132.32	123.70
26	BA	1572	A	C5-C6-N6	10.78	132.32	123.70
26	BA	1608	A	C5-C6-N6	10.78	132.32	123.70
26	BA	176	A	C5-C6-N6	10.78	132.32	123.70
26	BA	191	A	C5-C6-N6	10.77	132.32	123.70
1	AA	901	A	N7-C8-N9	-10.77	108.41	113.80
26	BA	1073	A	C5-C6-N6	10.77	132.32	123.70
1	AA	32	A	C5-C6-N6	10.77	132.31	123.70
26	BA	190	A	C5-C6-N6	10.77	132.32	123.70
1	AA	959	A	C5-C6-N6	10.77	132.31	123.70
26	BA	753	A	C5-C6-N6	10.77	132.31	123.70
26	BA	2094	A	C5-C6-N6	10.77	132.31	123.70
26	BA	1070	A	C5-C6-N6	10.77	132.31	123.70
26	BA	1504	A	C5-C6-N6	10.77	132.31	123.70
26	BA	1548	A	C5-C6-N6	10.77	132.31	123.70
26	BA	1866	A	C5-C6-N6	10.77	132.31	123.70
26	BA	2205	A	C5-C6-N6	10.77	132.31	123.70
26	BA	255	A	C5-C6-N6	10.76	132.31	123.70
26	BA	2778	A	C5-C6-N6	10.76	132.31	123.70
26	BA	74	A	C5-C6-N6	10.76	132.31	123.70
26	BA	447	A	C5-C6-N6	10.76	132.31	123.70
26	BA	2706	A	C5-C6-N6	10.76	132.31	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	152	A	C5-C6-N6	10.76	132.31	123.70
26	BA	661	A	C5-C6-N6	10.76	132.31	123.70
26	BA	1494	A	C5-C6-N6	10.76	132.31	123.70
26	BA	1169	A	C5-C6-N6	10.76	132.30	123.70
26	BA	2336	A	C5-C6-N6	10.76	132.30	123.70
1	AA	1339	A	C5-C6-N6	10.75	132.30	123.70
25	AY	9	A	C5-C6-N6	10.75	132.30	123.70
26	BA	173	A	C5-C6-N6	10.75	132.30	123.70
1	AA	864	A	C5-C6-N6	10.75	132.30	123.70
26	BA	1553	A	C5-C6-N6	10.75	132.30	123.70
26	BA	2765	A	C5-C6-N6	10.75	132.30	123.70
26	BA	1077	A	C5-C6-N6	10.75	132.30	123.70
1	AA	908	A	C5-C6-N6	10.75	132.30	123.70
26	BA	1090	A	C5-C6-N6	10.75	132.30	123.70
26	BA	1637	A	C5-C6-N6	10.75	132.30	123.70
26	BA	1969	A	C5-C6-N6	10.75	132.30	123.70
26	BA	1938	A	C5-C6-N6	10.74	132.30	123.70
1	AA	563	A	C5-C6-N6	10.74	132.29	123.70
26	BA	528	A	N7-C8-N9	-10.74	108.43	113.80
26	BA	532	A	N3-C4-C5	-10.74	119.28	126.80
27	BB	66	A	C5-C6-N6	10.74	132.29	123.70
1	AA	1219	A	C5-C6-N6	10.74	132.29	123.70
25	AY	6	A	C5-C6-N6	10.74	132.29	123.70
27	BB	50	A	C5-C6-N6	10.74	132.29	123.70
1	AA	460	A	C5-C6-N6	10.73	132.29	123.70
1	AA	743	A	C5-C6-N6	10.73	132.29	123.70
26	BA	2430	A	N7-C8-N9	-10.73	108.43	113.80
26	BA	2776	A	C5-C6-N6	10.73	132.29	123.70
1	AA	1418	A	C5-C6-N6	10.73	132.29	123.70
1	AA	33	A	C5-C6-N6	10.73	132.28	123.70
1	AA	435	A	C5-C6-N6	10.73	132.28	123.70
1	AA	539	A	C5-C6-N6	10.73	132.28	123.70
1	AA	706	A	C5-C6-N6	10.73	132.29	123.70
1	AA	1021	A	C5-C6-N6	10.73	132.28	123.70
1	AA	1318	A	C5-C6-N6	10.73	132.28	123.70
26	BA	2014	A	C5-C6-N6	10.73	132.28	123.70
26	BA	2088	A	C5-C6-N6	10.73	132.28	123.70
27	BB	45	A	C5-C6-N6	10.72	132.28	123.70
1	AA	1483	A	C5-C6-N6	10.72	132.28	123.70
26	BA	1571	A	C5-C6-N6	10.72	132.28	123.70
26	BA	917	A	C5-C6-N6	10.72	132.27	123.70
26	BA	925	A	C5-C6-N6	10.72	132.27	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1676	A	C5-C6-N6	10.72	132.28	123.70
26	BA	1784	A	C5-C6-N6	10.72	132.27	123.70
26	BA	2287	A	N3-C4-C5	-10.72	119.30	126.80
26	BA	1603	A	C5-C6-N6	10.71	132.27	123.70
26	BA	471	A	C5-C6-N6	10.71	132.27	123.70
26	BA	2297	A	C5-C6-N6	10.71	132.27	123.70
26	BA	633	A	N7-C8-N9	-10.70	108.45	113.80
26	BA	2430	A	C5-C6-N6	10.70	132.26	123.70
26	BA	64	A	C5-C6-N6	10.70	132.26	123.70
26	BA	470	A	C5-C6-N6	10.70	132.26	123.70
1	AA	1508	A	C5-C6-N6	10.70	132.26	123.70
26	BA	1496	A	C5-C6-N6	10.70	132.26	123.70
26	BA	1669	A	C5-C6-N6	10.70	132.26	123.70
26	BA	1805	A	C5-C6-N6	10.70	132.26	123.70
1	AA	1374	A	C5-C6-N6	10.70	132.26	123.70
26	BA	1614	A	C5-C6-N6	10.70	132.26	123.70
1	AA	482	A	C5-C6-N6	10.69	132.25	123.70
24	AX	23	A	C5-C6-N6	10.69	132.25	123.70
26	BA	131	A	C5-C6-N6	10.69	132.25	123.70
26	BA	2013	A	C5-C6-N6	10.69	132.25	123.70
26	BA	2273	A	C5-C6-N6	10.69	132.25	123.70
26	BA	2284	A	C5-C6-N6	10.69	132.25	123.70
26	BA	1634	A	C5-C6-N6	10.69	132.25	123.70
26	BA	2856	A	C5-C6-N6	10.69	132.25	123.70
1	AA	640	A	C5-C6-N6	10.69	132.25	123.70
1	AA	192	A	C5-C6-N6	10.68	132.25	123.70
26	BA	743	A	C5-C6-N6	10.68	132.25	123.70
26	BA	1791	A	C5-C6-N6	10.68	132.25	123.70
1	AA	1324	A	C5-C6-N6	10.68	132.25	123.70
26	BA	705	A	C5-C6-N6	10.68	132.24	123.70
26	BA	1301	A	N3-C4-C5	-10.68	119.33	126.80
26	BA	2169	A	C5-C6-N6	10.68	132.24	123.70
1	AA	814	A	C5-C6-N6	10.68	132.24	123.70
26	BA	2837	A	C5-C6-N6	10.67	132.24	123.70
1	AA	1476	A	C5-C6-N6	10.67	132.23	123.70
26	BA	532	A	C5-C6-N6	10.67	132.23	123.70
26	BA	1029	A	C5-C6-N6	10.67	132.23	123.70
26	BA	2547	A	C5-C6-N6	10.67	132.23	123.70
1	AA	162	A	C5-C6-N6	10.66	132.23	123.70
26	BA	1301	A	N7-C8-N9	-10.66	108.47	113.80
26	BA	2407	A	C5-C6-N6	10.66	132.23	123.70
1	AA	938	A	C5-C6-N6	10.65	132.22	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2748	A	C5-C6-N6	10.65	132.22	123.70
1	AA	432	A	C5-C6-N6	10.65	132.22	123.70
1	AA	873	A	C5-C6-N6	10.65	132.22	123.70
26	BA	63	A	C5-C6-N6	10.65	132.22	123.70
26	BA	1829	A	C5-C6-N6	10.65	132.22	123.70
26	BA	2080	A	C5-C6-N6	10.64	132.21	123.70
1	AA	270	A	C5-C6-N6	10.64	132.21	123.70
1	AA	451	A	C5-C6-N6	10.64	132.21	123.70
1	AA	430	A	C5-C6-N6	10.64	132.21	123.70
26	BA	415	A	C5-C6-N6	10.64	132.21	123.70
26	BA	1395	A	C5-C6-N6	10.64	132.21	123.70
26	BA	2516	A	C5-C6-N6	10.64	132.21	123.70
1	AA	872	A	C5-C6-N6	10.63	132.21	123.70
26	BA	845	A	C5-C6-N6	10.63	132.21	123.70
26	BA	1387	A	C5-C6-N6	10.63	132.20	123.70
26	BA	1745	A	C5-C6-N6	10.63	132.21	123.70
1	AA	371	A	C5-C6-N6	10.63	132.20	123.70
26	BA	677	A	C5-C6-N6	10.63	132.20	123.70
1	AA	1340	A	C5-C6-N6	10.62	132.20	123.70
1	AA	1429	A	C5-C6-N6	10.62	132.20	123.70
1	AA	190	A	C5-C6-N6	10.62	132.20	123.70
1	AA	1022	A	C5-C6-N6	10.62	132.20	123.70
1	AA	329	A	C5-C6-N6	10.62	132.20	123.70
26	BA	582	A	C5-C6-N6	10.62	132.19	123.70
26	BA	1669	A	N7-C8-N9	-10.62	108.49	113.80
25	AY	66	A	C5-C6-N6	10.62	132.19	123.70
26	BA	1241	A	C5-C6-N6	10.62	132.19	123.70
1	AA	300	A	C5-C6-N6	10.61	132.19	123.70
1	AA	935	A	C5-C6-N6	10.61	132.19	123.70
26	BA	2386	A	C5-C6-N6	10.61	132.19	123.70
26	BA	794	A	C5-C6-N6	10.61	132.19	123.70
26	BA	1970	A	C5-C6-N6	10.61	132.19	123.70
26	BA	52	A	C5-C6-N6	10.61	132.19	123.70
1	AA	478	A	C5-C6-N6	10.61	132.19	123.70
26	BA	1353	A	C5-C6-N6	10.61	132.19	123.70
26	BA	1899	A	C5-C6-N6	10.61	132.18	123.70
26	BA	2184	A	C5-C6-N6	10.60	132.18	123.70
26	BA	2267	A	C5-C6-N6	10.60	132.18	123.70
1	AA	53	A	C5-C6-N6	10.59	132.17	123.70
1	AA	1357	A	C5-C6-N6	10.59	132.17	123.70
1	AA	1468	A	C5-C6-N6	10.59	132.17	123.70
26	BA	2461	A	C5-C6-N6	10.59	132.17	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	513	A	C5-C6-N6	10.58	132.17	123.70
26	BA	2765	A	N3-C4-C5	-10.58	119.39	126.80
26	BA	1213	A	C5-C6-N6	10.58	132.16	123.70
26	BA	2267	A	N3-C4-C5	-10.58	119.39	126.80
1	AA	746	A	C5-C6-N6	10.58	132.16	123.70
26	BA	2766	A	C5-C6-N6	10.58	132.16	123.70
26	BA	2054	A	C5-C6-N6	10.58	132.16	123.70
1	AA	865	A	C5-C6-N6	10.58	132.16	123.70
26	BA	750	A	C5-C6-N6	10.58	132.16	123.70
26	BA	1810	A	C5-C6-N6	10.57	132.16	123.70
26	BA	685	A	C5-C6-N6	10.57	132.15	123.70
26	BA	2142	A	C5-C6-N6	10.56	132.15	123.70
26	BA	2799	A	C5-C6-N6	10.56	132.15	123.70
26	BA	2171	A	C5-C6-N6	10.56	132.15	123.70
26	BA	231	A	C5-C6-N6	10.55	132.14	123.70
26	BA	1244	A	C5-C6-N6	10.55	132.14	123.70
26	BA	572	A	C5-C6-N6	10.54	132.13	123.70
26	BA	2077	A	N3-C4-C5	-10.54	119.42	126.80
1	AA	356	A	C5-C6-N6	10.52	132.11	123.70
26	BA	2471	A	C5-C6-N6	10.51	132.11	123.70
24	AX	24	A	C5-C6-N6	10.51	132.11	123.70
26	BA	2287	A	C5-C6-N6	10.51	132.11	123.70
26	BA	503	A	C5-C6-N6	10.50	132.10	123.70
1	AA	55	A	C5-C6-N6	10.50	132.10	123.70
26	BA	430	A	C5-C6-N6	10.50	132.10	123.70
26	BA	2297	A	N3-C4-C5	-10.50	119.45	126.80
26	BA	756	A	C5-C6-N6	10.49	132.09	123.70
1	AA	923	A	C5-C6-N6	10.49	132.09	123.70
1	AA	1350	A	C5-C6-N6	10.49	132.09	123.70
1	AA	1152	A	C5-C6-N6	10.49	132.09	123.70
1	AA	546	A	C5-C6-N6	10.48	132.09	123.70
26	BA	1532	A	C5-C6-N6	10.48	132.09	123.70
1	AA	901	A	C5-C6-N6	10.48	132.09	123.70
26	BA	1549	A	C5-C6-N6	10.48	132.08	123.70
26	BA	819	A	C5-C6-N6	10.47	132.08	123.70
26	BA	449	A	C5-C6-N6	10.47	132.08	123.70
26	BA	1276	A	C5-C6-N6	10.47	132.07	123.70
26	BA	1664	A	C5-C6-N6	10.46	132.06	123.70
26	BA	2114	A	N7-C8-N9	-10.45	108.58	113.80
1	AA	563	A	N3-C4-C5	-10.44	119.49	126.80
26	BA	2459	A	C5-C6-N6	10.44	132.05	123.70
26	BA	960	A	C5-C6-N6	10.44	132.05	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2191	A	C5-C6-N6	10.44	132.05	123.70
23	AW	26	A	C5-C6-N6	10.44	132.05	123.70
26	BA	1021	A	N3-C4-C5	-10.43	119.50	126.80
1	AA	983	A	N7-C8-N9	-10.42	108.59	113.80
26	BA	644	A	C5-C6-N6	10.41	132.03	123.70
26	BA	2335	A	C5-C6-N6	10.39	132.02	123.70
1	AA	1507	A	C5-C6-N6	10.39	132.01	123.70
27	BB	59	A	N3-C4-C5	-10.39	119.53	126.80
26	BA	933	A	C5-C6-N6	10.38	132.00	123.70
26	BA	1570	A	C5-C6-N6	10.38	132.01	123.70
26	BA	2725	A	C5-C6-N6	10.38	132.00	123.70
1	AA	1363	A	C5-C6-N6	10.38	132.00	123.70
1	AA	1005	A	C5-C6-N6	10.38	132.00	123.70
26	BA	1535	A	N3-C4-C5	-10.38	119.53	126.80
1	AA	1167	A	N3-C4-C5	-10.37	119.54	126.80
1	AA	502	A	C5-C6-N6	10.37	131.99	123.70
1	AA	872	A	N3-C4-C5	-10.37	119.54	126.80
26	BA	2675	A	C5-C6-N6	10.36	131.99	123.70
23	AW	23	A	C5-C6-N6	10.34	131.97	123.70
26	BA	2800	A	C5-C6-N6	10.34	131.97	123.70
26	BA	1970	A	N3-C4-C5	-10.34	119.56	126.80
1	AA	495	A	C5-C6-N6	10.33	131.96	123.70
1	AA	977	A	N3-C4-C5	-10.33	119.57	126.80
1	AA	116	A	N3-C4-C5	-10.32	119.58	126.80
26	BA	330	A	C5-C6-N6	10.31	131.95	123.70
1	AA	1157	A	C5-C6-N6	10.30	131.94	123.70
26	BA	689	A	C5-C6-N6	10.30	131.94	123.70
1	AA	1044	A	C5-C6-N6	10.30	131.94	123.70
1	AA	608	A	C5-C6-N6	10.30	131.94	123.70
26	BA	2662	A	C5-C6-N6	10.29	131.93	123.70
1	AA	1102	A	C5-C6-N6	10.28	131.93	123.70
26	BA	1570	A	N3-C4-C5	-10.28	119.61	126.80
26	BA	278	A	N7-C8-N9	-10.27	108.66	113.80
26	BA	633	A	N3-C4-C5	-10.27	119.61	126.80
26	BA	633	A	C5-C6-N6	10.27	131.91	123.70
26	BA	863	A	C5-C6-N6	10.25	131.90	123.70
26	BA	1664	A	N3-C4-C5	-10.25	119.63	126.80
26	BA	2766	A	N3-C4-C5	-10.24	119.63	126.80
26	BA	1583	A	N3-C4-C5	-10.24	119.63	126.80
1	AA	98	A	N3-C4-C5	-10.24	119.63	126.80
26	BA	196	A	N3-C4-C5	-10.24	119.63	126.80
26	BA	142	A	C5-C6-N6	10.23	131.88	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	404	A	N3-C4-C5	-10.22	119.64	126.80
1	AA	994	A	N3-C4-C5	-10.21	119.66	126.80
26	BA	2062	A	N3-C4-C5	-10.20	119.66	126.80
26	BA	56	A	N3-C4-C5	-10.20	119.66	126.80
26	BA	599	A	C5-C6-N6	10.20	131.86	123.70
26	BA	845	A	N3-C4-C5	-10.20	119.66	126.80
26	BA	933	A	N3-C4-C5	-10.19	119.67	126.80
23	AW	23	A	N3-C4-C5	-10.19	119.67	126.80
26	BA	330	A	N3-C4-C5	-10.18	119.68	126.80
1	AA	1005	A	N3-C4-C5	-10.16	119.69	126.80
1	AA	1102	A	N3-C4-C5	-10.16	119.69	126.80
1	AA	539	A	N3-C4-C5	-10.16	119.69	126.80
26	BA	1490	A	N3-C4-C5	-10.16	119.69	126.80
27	BB	73	A	N3-C4-C5	-10.16	119.69	126.80
26	BA	960	A	N3-C4-C5	-10.15	119.69	126.80
26	BA	2560	A	N3-C4-C5	-10.15	119.69	126.80
1	AA	1044	A	N3-C4-C5	-10.14	119.70	126.80
26	BA	142	A	N3-C4-C5	-10.14	119.70	126.80
26	BA	362	A	N3-C4-C5	-10.14	119.70	126.80
1	AA	1299	A	N3-C4-C5	-10.14	119.70	126.80
26	BA	5	A	N3-C4-C5	-10.13	119.71	126.80
1	AA	706	A	N3-C4-C5	-10.13	119.71	126.80
26	BA	819	A	N3-C4-C5	-10.13	119.71	126.80
26	BA	384	A	N3-C4-C5	-10.12	119.71	126.80
26	BA	599	A	N3-C4-C5	-10.12	119.71	126.80
26	BA	514	A	N3-C4-C5	-10.12	119.72	126.80
26	BA	2211	A	N3-C4-C5	-10.12	119.72	126.80
1	AA	918	A	N3-C4-C5	-10.12	119.72	126.80
26	BA	1088	A	N3-C4-C5	-10.12	119.72	126.80
26	BA	1901	A	N3-C4-C5	-10.11	119.72	126.80
1	AA	408	A	N7-C8-N9	-10.11	108.75	113.80
1	AA	397	A	C5-C6-N6	10.11	131.79	123.70
26	BA	572	A	N3-C4-C5	-10.10	119.73	126.80
1	AA	478	A	N3-C4-C5	-10.09	119.74	126.80
1	AA	1363	A	N3-C4-C5	-10.09	119.74	126.80
26	BA	2560	A	C5-C6-N6	10.09	131.77	123.70
26	BA	1494	A	N3-C4-C5	-10.09	119.74	126.80
26	BA	644	A	N3-C4-C5	-10.08	119.74	126.80
27	BB	15	A	N3-C4-C5	-10.08	119.74	126.80
26	BA	52	A	N3-C4-C5	-10.08	119.74	126.80
26	BA	160	A	N3-C4-C5	-10.08	119.74	126.80
1	AA	546	A	N3-C4-C5	-10.08	119.75	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	901	A	N3-C4-C5	-10.07	119.75	126.80
26	BA	513	A	N3-C4-C5	-10.07	119.75	126.80
1	AA	1332	A	N3-C4-C5	-10.07	119.75	126.80
26	BA	231	A	N3-C4-C5	-10.06	119.76	126.80
26	BA	131	A	N3-C4-C5	-10.06	119.76	126.80
26	BA	675	A	N3-C4-C5	-10.05	119.76	126.80
26	BA	1784	A	N3-C4-C5	-10.05	119.76	126.80
26	BA	2407	A	N3-C4-C5	-10.05	119.77	126.80
1	AA	448	A	N3-C4-C5	-10.05	119.77	126.80
26	BA	1829	A	N3-C4-C5	-10.04	119.77	126.80
26	BA	2516	A	N3-C4-C5	-10.04	119.77	126.80
26	BA	2662	A	N3-C4-C5	-10.04	119.77	126.80
26	BA	1000	A	N3-C4-C5	-10.04	119.77	126.80
26	BA	1635	A	N3-C4-C5	-10.03	119.78	126.80
1	AA	579	A	N3-C4-C5	-10.03	119.78	126.80
26	BA	1866	A	N3-C4-C5	-10.03	119.78	126.80
26	BA	2665	A	N3-C4-C5	-10.03	119.78	126.80
23	AW	26	A	N3-C4-C5	-10.03	119.78	126.80
26	BA	1899	A	N3-C4-C5	-10.03	119.78	126.80
26	BA	56	A	C5-C6-N6	10.02	131.72	123.70
26	BA	1276	A	N3-C4-C5	-10.02	119.78	126.80
26	BA	1353	A	N3-C4-C5	-10.02	119.78	126.80
26	BA	2335	A	N3-C4-C5	-10.02	119.78	126.80
1	AA	1418	A	N3-C4-C5	-10.02	119.79	126.80
26	BA	64	A	N3-C4-C5	-10.02	119.79	126.80
26	BA	1213	A	N3-C4-C5	-10.02	119.79	126.80
26	BA	2740	A	N3-C4-C5	-10.02	119.79	126.80
1	AA	1507	A	N3-C4-C5	-10.02	119.79	126.80
26	BA	471	A	N3-C4-C5	-10.02	119.79	126.80
26	BA	2461	A	N3-C4-C5	-10.02	119.79	126.80
1	AA	1225	A	N3-C4-C5	-10.01	119.79	126.80
26	BA	1086	A	N3-C4-C5	-10.01	119.79	126.80
1	AA	468	A	N3-C4-C5	-10.01	119.79	126.80
26	BA	449	A	N3-C4-C5	-10.01	119.79	126.80
26	BA	1553	A	N3-C4-C5	-10.01	119.79	126.80
26	BA	1919	A	N3-C4-C5	-10.01	119.79	126.80
26	BA	2518	A	N3-C4-C5	-10.01	119.79	126.80
26	BA	547	A	N3-C4-C5	-10.01	119.79	126.80
26	BA	756	A	N3-C4-C5	-10.01	119.79	126.80
26	BA	470	A	N3-C4-C5	-10.01	119.80	126.80
26	BA	654	A	N3-C4-C5	-10.00	119.80	126.80
26	BA	863	A	N3-C4-C5	-10.00	119.80	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2471	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	55	A	N3-C4-C5	-10.00	119.80	126.80
26	BA	917	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	356	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	743	A	N3-C4-C5	-9.99	119.81	126.80
26	BA	689	A	N3-C4-C5	-9.99	119.81	126.80
1	AA	509	A	N3-C4-C5	-9.99	119.81	126.80
1	AA	923	A	N3-C4-C5	-9.99	119.81	126.80
1	AA	1157	A	N3-C4-C5	-9.99	119.81	126.80
1	AA	435	A	N3-C4-C5	-9.99	119.81	126.80
26	BA	401	A	N3-C4-C5	-9.98	119.81	126.80
26	BA	794	A	N3-C4-C5	-9.98	119.81	126.80
26	BA	1395	A	N3-C4-C5	-9.98	119.81	126.80
26	BA	1469	A	N3-C4-C5	-9.98	119.81	126.80
1	AA	408	A	N3-C4-C5	-9.98	119.82	126.80
26	BA	2386	A	N3-C4-C5	-9.98	119.82	126.80
1	AA	487	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	938	A	N3-C4-C5	-9.97	119.82	126.80
26	BA	1787	A	N3-C4-C5	-9.97	119.82	126.80
26	BA	2327	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	1476	A	N3-C4-C5	-9.97	119.82	126.80
26	BA	750	A	N3-C4-C5	-9.97	119.82	126.80
26	BA	1365	A	N3-C4-C5	-9.97	119.82	126.80
26	BA	1392	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	162	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	190	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	270	A	N3-C4-C5	-9.97	119.82	126.80
23	AW	59	A	N3-C4-C5	-9.97	119.82	126.80
24	AX	23	A	N3-C4-C5	-9.97	119.82	126.80
26	BA	2657	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	640	A	N3-C4-C5	-9.97	119.82	126.80
26	BA	191	A	N3-C4-C5	-9.97	119.82	126.80
26	BA	152	A	N3-C4-C5	-9.96	119.82	126.80
26	BA	1287	A	N3-C4-C5	-9.96	119.83	126.80
26	BA	2823	A	N3-C4-C5	-9.96	119.83	126.80
26	BA	190	A	N3-C4-C5	-9.96	119.83	126.80
26	BA	2727	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	496	A	N3-C4-C5	-9.96	119.83	126.80
26	BA	299	A	N3-C4-C5	-9.96	119.83	126.80
26	BA	1189	A	N3-C4-C5	-9.96	119.83	126.80
26	BA	1496	A	N3-C4-C5	-9.96	119.83	126.80
26	BA	1608	A	N3-C4-C5	-9.96	119.83	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	910	A	N3-C4-C5	-9.96	119.83	126.80
26	BA	1048	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	389	A	N3-C4-C5	-9.95	119.83	126.80
1	AA	907	A	N3-C4-C5	-9.95	119.83	126.80
1	AA	694	A	N3-C4-C5	-9.95	119.83	126.80
1	AA	712	A	N3-C4-C5	-9.95	119.83	126.80
1	AA	1176	A	N3-C4-C5	-9.95	119.84	126.80
26	BA	173	A	N3-C4-C5	-9.95	119.83	126.80
26	BA	2051	A	N3-C4-C5	-9.95	119.83	126.80
26	BA	251	A	N3-C4-C5	-9.95	119.84	126.80
26	BA	374	A	N3-C4-C5	-9.95	119.83	126.80
26	BA	382	A	N3-C4-C5	-9.95	119.84	126.80
26	BA	693	A	N3-C4-C5	-9.95	119.84	126.80
26	BA	582	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	553	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	621	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	780	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	1468	A	N3-C4-C5	-9.94	119.84	126.80
26	BA	1809	A	N3-C4-C5	-9.94	119.84	126.80
26	BA	2163	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	329	A	N3-C4-C5	-9.94	119.84	126.80
24	AX	14	A	N3-C4-C5	-9.94	119.84	126.80
26	BA	2070	A	N3-C4-C5	-9.94	119.84	126.80
26	BA	2273	A	N3-C4-C5	-9.94	119.84	126.80
27	BB	29	A	N3-C4-C5	-9.94	119.84	126.80
27	BB	115	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	1531	A	N3-C4-C5	-9.93	119.85	126.80
25	AY	6	A	N3-C4-C5	-9.93	119.85	126.80
26	BA	1244	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	71	A	N3-C4-C5	-9.93	119.85	126.80
26	BA	1241	A	N3-C4-C5	-9.93	119.85	126.80
26	BA	1169	A	N3-C4-C5	-9.93	119.85	126.80
27	BB	57	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	1374	A	N3-C4-C5	-9.93	119.85	126.80
26	BA	255	A	N3-C4-C5	-9.93	119.85	126.80
26	BA	632	A	N3-C4-C5	-9.93	119.85	126.80
26	BA	1571	A	N3-C4-C5	-9.93	119.85	126.80
26	BA	2171	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	53	A	N3-C4-C5	-9.92	119.85	126.80
1	AA	373	A	N3-C4-C5	-9.92	119.85	126.80
1	AA	608	A	N3-C4-C5	-9.92	119.85	126.80
26	BA	2054	A	N3-C4-C5	-9.92	119.85	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	453	A	N3-C4-C5	-9.92	119.85	126.80
26	BA	802	A	N3-C4-C5	-9.92	119.85	126.80
26	BA	820	A	N3-C4-C5	-9.92	119.85	126.80
26	BA	1744	A	N3-C4-C5	-9.92	119.85	126.80
1	AA	873	A	N3-C4-C5	-9.92	119.86	126.80
26	BA	176	A	N3-C4-C5	-9.92	119.86	126.80
26	BA	2080	A	N3-C4-C5	-9.92	119.86	126.80
26	BA	2837	A	N3-C4-C5	-9.92	119.86	126.80
1	AA	1146	A	N3-C4-C5	-9.92	119.86	126.80
26	BA	2799	A	N3-C4-C5	-9.92	119.86	126.80
26	BA	1029	A	N3-C4-C5	-9.92	119.86	126.80
26	BA	1969	A	N3-C4-C5	-9.92	119.86	126.80
26	BA	2900	A	N3-C4-C5	-9.92	119.86	126.80
27	BB	53	A	N3-C4-C5	-9.92	119.86	126.80
1	AA	1357	A	N3-C4-C5	-9.91	119.86	126.80
24	AX	24	A	N3-C4-C5	-9.91	119.86	126.80
26	BA	182	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	1350	A	N3-C4-C5	-9.91	119.86	126.80
26	BA	1998	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	19	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	696	A	N3-C4-C5	-9.91	119.86	126.80
26	BA	233	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	814	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	1339	A	N3-C4-C5	-9.91	119.86	126.80
25	AY	69	A	N3-C4-C5	-9.91	119.86	126.80
26	BA	685	A	N3-C4-C5	-9.91	119.86	126.80
26	BA	2748	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	431	A	N3-C4-C5	-9.91	119.87	126.80
26	BA	2328	A	N3-C4-C5	-9.91	119.87	126.80
26	BA	2725	A	N3-C4-C5	-9.91	119.86	126.80
26	BA	2809	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	228	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	642	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	746	A	N3-C4-C5	-9.90	119.87	126.80
26	BA	346	A	N3-C4-C5	-9.90	119.87	126.80
26	BA	2547	A	N3-C4-C5	-9.90	119.87	126.80
26	BA	352	A	N3-C4-C5	-9.90	119.87	126.80
26	BA	2879	A	N3-C4-C5	-9.90	119.87	126.80
26	BA	706	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	949	A	N3-C4-C5	-9.90	119.87	126.80
26	BA	10	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	371	A	N3-C4-C5	-9.90	119.87	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1262	A	N3-C4-C5	-9.90	119.87	126.80
26	BA	2184	A	N3-C4-C5	-9.90	119.87	126.80
26	BA	2758	A	N3-C4-C5	-9.90	119.87	126.80
26	BA	2634	A	N3-C4-C5	-9.89	119.87	126.80
1	AA	908	A	N3-C4-C5	-9.89	119.88	126.80
26	BA	1084	A	N3-C4-C5	-9.89	119.87	126.80
26	BA	1103	A	N3-C4-C5	-9.89	119.88	126.80
26	BA	2352	A	N3-C4-C5	-9.89	119.87	126.80
27	BB	99	A	N3-C4-C5	-9.89	119.87	126.80
1	AA	98	A	C5-C6-N6	9.89	131.61	123.70
26	BA	2873	A	N3-C4-C5	-9.89	119.88	126.80
26	BA	753	A	N3-C4-C5	-9.89	119.88	126.80
26	BA	2459	A	N3-C4-C5	-9.89	119.88	126.80
26	BA	2366	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	313	A	N3-C4-C5	-9.88	119.88	126.80
26	BA	1597	A	N3-C4-C5	-9.88	119.88	126.80
26	BA	2706	A	N3-C4-C5	-9.88	119.88	126.80
24	AX	41	A	N3-C4-C5	-9.88	119.88	126.80
26	BA	705	A	N3-C4-C5	-9.88	119.88	126.80
26	BA	730	A	N3-C4-C5	-9.88	119.88	126.80
26	BA	1260	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	130	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	306	A	N3-C4-C5	-9.88	119.88	126.80
26	BA	1230	A	N3-C4-C5	-9.88	119.88	126.80
26	BA	1453	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	119	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	1429	A	N3-C4-C5	-9.88	119.89	126.80
26	BA	219	A	N3-C4-C5	-9.88	119.89	126.80
26	BA	1637	A	N3-C4-C5	-9.88	119.88	126.80
26	BA	2378	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	236	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	1004	A	N3-C4-C5	-9.88	119.89	126.80
26	BA	1847	A	N3-C4-C5	-9.88	119.89	126.80
26	BA	1548	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	460	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	831	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	864	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	71	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	2412	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	2887	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	443	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	715	A	N3-C4-C5	-9.87	119.89	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	860	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	1340	A	N3-C4-C5	-9.87	119.89	126.80
24	AX	3	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	144	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	1028	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	2587	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	6	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	195	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	279	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	595	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	787	A	N3-C4-C5	-9.86	119.89	126.80
23	AW	58	A	N3-C4-C5	-9.86	119.89	126.80
25	AY	23	A	N3-C4-C5	-9.86	119.89	126.80
26	BA	348	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	1268	A	N3-C4-C5	-9.86	119.89	126.80
26	BA	1634	A	N3-C4-C5	-9.87	119.89	126.80
26	BA	849	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	1127	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	1214	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	1264	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	300	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	1152	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	1252	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	423	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	1499	A	N3-C4-C5	-9.86	119.90	126.80
24	AX	26	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	1810	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	2014	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	2856	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	167	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	2205	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	28	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	197	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	428	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	833	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	1387	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	2564	A	N3-C4-C5	-9.86	119.90	126.80
26	BA	2088	A	N3-C4-C5	-9.85	119.90	126.80
1	AA	33	A	N3-C4-C5	-9.85	119.90	126.80
1	AA	1483	A	N3-C4-C5	-9.85	119.90	126.80
26	BA	1054	A	N3-C4-C5	-9.85	119.90	126.80
26	BA	2721	A	N3-C4-C5	-9.85	119.90	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	704	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	1349	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	1360	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	792	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	925	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	1504	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	1618	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	1260	A	C5-C6-N6	9.85	131.58	123.70
26	BA	1549	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	2082	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	2173	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	2800	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	1508	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	1307	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	2850	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	408	A	C5-C6-N6	9.85	131.58	123.70
1	AA	1219	A	N3-C4-C5	-9.85	119.91	126.80
25	AY	66	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	472	A	N3-C4-C5	-9.85	119.91	126.80
26	BA	1773	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	192	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1022	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	203	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	501	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1171	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1430	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	391	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	716	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	943	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	1269	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	959	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	1579	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	2311	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	2757	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	2792	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	2142	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	2191	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	2212	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	600	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1396	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	101	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	1144	A	N3-C4-C5	-9.84	119.91	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2094	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	2813	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	59	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	482	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1261	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	415	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	2013	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	2531	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	223	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	111	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	784	A	N3-C4-C5	-9.84	119.92	126.80
1	AA	1036	A	N3-C4-C5	-9.84	119.92	126.80
1	AA	1362	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1503	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	1927	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	2134	A	N3-C4-C5	-9.84	119.91	126.80
26	BA	718	A	N3-C4-C5	-9.84	119.92	126.80
26	BA	1966	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	32	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	320	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	363	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	522	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	1591	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	2095	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	695	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	49	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	541	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	1090	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	1762	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	1858	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	2635	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	1952	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	2476	A	N3-C4-C5	-9.83	119.92	126.80
27	BB	52	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	751	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	1095	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	1603	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	303	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	782	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	825	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	878	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	1093	A	N3-C4-C5	-9.83	119.92	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1191	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	1377	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	1027	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	1050	A	N3-C4-C5	-9.83	119.92	126.80
26	BA	1328	A	N3-C4-C5	-9.83	119.92	126.80
23	AW	73	A	N3-C4-C5	-9.82	119.92	126.80
25	AY	21	A	N3-C4-C5	-9.82	119.92	126.80
26	BA	256	A	N3-C4-C5	-9.82	119.92	126.80
26	BA	1247	A	N3-C4-C5	-9.82	119.92	126.80
26	BA	2042	A	N3-C4-C5	-9.82	119.92	126.80
26	BA	2439	A	N3-C4-C5	-9.82	119.92	126.80
26	BA	14	A	N3-C4-C5	-9.82	119.92	126.80
26	BA	492	A	N3-C4-C5	-9.82	119.92	126.80
26	BA	1876	A	N3-C4-C5	-9.82	119.92	126.80
26	BA	735	A	N3-C4-C5	-9.82	119.92	126.80
1	AA	65	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	958	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	1105	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	1169	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	1324	A	N3-C4-C5	-9.82	119.93	126.80
26	BA	181	A	N3-C4-C5	-9.82	119.93	126.80
26	BA	1272	A	N3-C4-C5	-9.82	119.93	126.80
26	BA	2675	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	149	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	900	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	1311	A	N3-C4-C5	-9.82	119.93	126.80
23	AW	9	A	N3-C4-C5	-9.82	119.93	126.80
26	BA	1098	A	N3-C4-C5	-9.82	119.93	126.80
23	AW	41	A	N3-C4-C5	-9.82	119.93	126.80
26	BA	1151	A	N3-C4-C5	-9.82	119.93	126.80
26	BA	1226	A	N3-C4-C5	-9.82	119.93	126.80
26	BA	504	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	592	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	2711	A	N3-C4-C5	-9.81	119.93	126.80
22	AV	20	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	2778	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	2821	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	630	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	845	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	877	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	2776	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	344	A	N3-C4-C5	-9.81	119.93	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1046	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	2015	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	2733	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	1269	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	1456	A	N3-C4-C5	-9.81	119.94	126.80
25	AY	26	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	118	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	429	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	666	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	972	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	2497	A	N3-C4-C5	-9.81	119.93	126.80
26	BA	1470	A	N3-C4-C5	-9.81	119.94	126.80
26	BA	1889	A	N3-C4-C5	-9.81	119.94	126.80
26	BA	2411	A	N3-C4-C5	-9.81	119.94	126.80
26	BA	2541	A	N3-C4-C5	-9.81	119.94	126.80
1	AA	675	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	716	A	N3-C4-C5	-9.81	119.94	126.80
1	AA	728	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1306	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	722	A	N3-C4-C5	-9.81	119.94	126.80
23	AW	38	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	309	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	602	A	N3-C4-C5	-9.81	119.94	126.80
26	BA	661	A	N3-C4-C5	-9.81	119.94	126.80
26	BA	866	A	N3-C4-C5	-9.81	119.94	126.80
26	BA	2284	A	N3-C4-C5	-9.81	119.94	126.80
26	BA	2468	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	2700	A	N3-C4-C5	-9.81	119.94	126.80
26	BA	103	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	631	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	1528	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	1745	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	1746	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	2886	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	2820	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	935	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	439	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	804	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1280	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1346	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	44	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	218	A	N3-C4-C5	-9.80	119.94	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1367	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	1505	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	1641	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	2317	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	1532	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	447	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	635	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	906	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	964	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1014	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1021	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1433	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1446	A	N3-C4-C5	-9.80	119.94	126.80
25	AY	35	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	13	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	222	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	1572	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	2101	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	189	A	N3-C4-C5	-9.79	119.94	126.80
1	AA	523	A	N3-C4-C5	-9.79	119.94	126.80
1	AA	655	A	N3-C4-C5	-9.79	119.94	126.80
1	AA	1319	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	430	A	N3-C4-C5	-9.80	119.94	126.80
26	BA	1327	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1080	A	N3-C4-C5	-9.79	119.94	126.80
26	BA	613	A	N3-C4-C5	-9.79	119.94	126.80
26	BA	861	A	N3-C4-C5	-9.79	119.94	126.80
26	BA	918	A	N3-C4-C5	-9.79	119.94	126.80
26	BA	1274	A	N3-C4-C5	-9.79	119.94	126.80
26	BA	2705	A	N3-C4-C5	-9.79	119.94	126.80
1	AA	174	A	N3-C4-C5	-9.79	119.94	126.80
1	AA	414	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	629	A	N3-C4-C5	-9.79	119.94	126.80
1	AA	1042	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	345	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	739	A	N3-C4-C5	-9.79	119.94	126.80
26	BA	1302	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	1384	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	1885	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	1977	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	1035	A	N3-C4-C5	-9.79	119.95	126.80
22	AV	17	A	N3-C4-C5	-9.79	119.95	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	28	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	325	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	461	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	510	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	1375	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	94	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	165	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	217	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	282	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	342	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	482	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	984	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	1321	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	1383	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	1672	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	1717	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	2198	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	2077	A	C5-C6-N6	9.79	131.53	123.70
26	BA	2602	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	2899	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	432	A	N3-C4-C5	-9.79	119.95	126.80
23	AW	21	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	1012	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	347	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	556	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	1111	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1194	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1434	A	N3-C4-C5	-9.79	119.95	126.80
26	BA	1848	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	2434	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	2530	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	451	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	1251	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1502	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	199	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	607	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1008	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1632	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1853	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	2030	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	2392	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	353	A	N3-C4-C5	-9.78	119.95	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	366	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	382	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	226	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	332	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	721	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	975	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1067	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	825	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	1197	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	909	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	996	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1069	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1544	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1701	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	1791	A	N3-C4-C5	-9.78	119.95	126.80
26	BA	2369	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	81	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	914	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	1016	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	1318	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	1534	A	N3-C4-C5	-9.78	119.96	126.80
23	AW	69	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	172	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	1366	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	1477	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	1143	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	1175	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	1877	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	1936	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	1938	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	2288	A	N3-C4-C5	-9.78	119.96	126.80
26	BA	2333	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	532	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	573	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	596	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	74	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	402	A	N3-C4-C5	-9.77	119.96	126.80
27	BB	39	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	8	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	560	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	676	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	968	A	N3-C4-C5	-9.77	119.96	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	58	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	412	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	1676	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	1783	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	2170	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	2241	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	2268	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	2750	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	161	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	181	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	892	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	1254	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	149	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	432	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	1126	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	649	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	794	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	146	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	502	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	699	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	743	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	900	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	1354	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	1508	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	1596	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	1650	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	1872	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	2005	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	2117	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	2199	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	2761	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	2425	A	N3-C4-C5	-9.77	119.96	126.80
27	BB	94	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	72	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	129	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	777	A	N3-C4-C5	-9.77	119.96	126.80
22	AV	19	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	1373	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	160	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	946	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	1019	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	216	A	N3-C4-C5	-9.77	119.97	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	422	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	979	A	N3-C4-C5	-9.77	119.96	126.80
26	BA	1070	A	N3-C4-C5	-9.77	119.97	126.80
26	BA	2893	A	N3-C4-C5	-9.77	119.96	126.80
27	BB	101	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	109	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	155	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	262	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	2781	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	1431	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	1502	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	262	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	941	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1009	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1433	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1439	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	2052	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	2336	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	2433	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	768	A	N3-C4-C5	-9.76	119.97	126.80
22	AV	22	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1665	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	865	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1679	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	2003	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	727	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1981	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	781	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	1428	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	95	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	460	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	505	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	670	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1336	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1640	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	2377	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	2660	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	980	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1089	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1403	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	1802	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	2670	A	N3-C4-C5	-9.76	119.97	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2753	A	N3-C4-C5	-9.76	119.97	126.80
26	BA	2810	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	807	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	1274	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	1580	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	1871	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	205	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	673	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	1204	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	344	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	508	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	734	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	1495	A	N3-C4-C5	-9.75	119.97	126.80
27	BB	59	A	C5-C6-N6	9.75	131.50	123.70
1	AA	120	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	152	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	702	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	1110	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	1434	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	19	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	563	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	1010	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	244	A	N3-C4-C5	-9.75	119.98	126.80
26	BA	892	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	2346	A	N3-C4-C5	-9.75	119.97	126.80
27	BB	119	A	N3-C4-C5	-9.75	119.97	126.80
26	BA	1342	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	465	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	715	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	1398	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	1441	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	1480	A	N3-C4-C5	-9.75	119.98	126.80
24	AX	21	A	N3-C4-C5	-9.75	119.98	126.80
26	BA	1801	A	N3-C4-C5	-9.75	119.98	126.80
25	AY	41	A	N3-C4-C5	-9.75	119.98	126.80
26	BA	368	A	N3-C4-C5	-9.75	119.98	126.80
26	BA	478	A	N3-C4-C5	-9.75	119.98	126.80
26	BA	590	A	N3-C4-C5	-9.75	119.98	126.80
26	BA	608	A	N3-C4-C5	-9.75	119.98	126.80
26	BA	643	A	N3-C4-C5	-9.75	119.98	126.80
26	BA	1039	A	N3-C4-C5	-9.75	119.98	126.80
26	BA	1609	A	N3-C4-C5	-9.75	119.98	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1698	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	2	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	383	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1111	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1196	A	N3-C4-C5	-9.74	119.98	126.80
24	AX	58	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	7	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	572	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	749	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1465	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	503	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	2281	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	371	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	616	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	1678	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	2058	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	2381	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	274	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	959	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1179	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1271	A	N3-C4-C5	-9.74	119.98	126.80
25	AY	14	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	479	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	896	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	1020	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	1085	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	1525	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	2060	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	2632	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	2738	A	N3-C4-C5	-9.74	119.98	126.80
27	BB	109	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	441	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	648	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	753	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1046	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1236	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	199	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	789	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	928	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	1393	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	1503	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	1754	A	N3-C4-C5	-9.74	119.98	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2227	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	2270	A	N3-C4-C5	-9.74	119.98	126.80
26	BA	2851	A	N3-C4-C5	-9.74	119.98	126.80
27	BB	78	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1163	A	N3-C4-C5	-9.73	119.98	126.80
26	BA	294	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	1180	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	1519	A	N3-C4-C5	-9.73	119.99	126.80
25	AY	9	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	272	A	N3-C4-C5	-9.73	119.98	126.80
26	BA	1552	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	2406	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	2654	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	2749	A	N3-C4-C5	-9.73	119.98	126.80
26	BA	2872	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	288	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	559	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	575	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	1431	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	583	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	663	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	1082	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	911	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	1805	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	2158	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	2309	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	1188	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	1156	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	2169	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	1368	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	528	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	78	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	1287	A	N3-C4-C5	-9.73	119.99	126.80
24	AX	76	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	1096	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	1912	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	2882	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	793	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	1308	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	1569	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	1722	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	1789	A	N3-C4-C5	-9.73	119.99	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1819	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	2426	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	2453	A	N3-C4-C5	-9.73	119.99	126.80
26	BA	2860	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	747	A	N3-C4-C5	-9.72	119.99	126.80
1	AA	1288	A	N3-C4-C5	-9.72	119.99	126.80
26	BA	2577	A	N3-C4-C5	-9.72	119.99	126.80
1	AA	816	A	N3-C4-C5	-9.72	119.99	126.80
26	BA	270	A	N3-C4-C5	-9.72	119.99	126.80
26	BA	626	A	N3-C4-C5	-9.72	119.99	126.80
26	BA	899	A	N3-C4-C5	-9.72	119.99	126.80
26	BA	1711	A	N3-C4-C5	-9.72	119.99	126.80
1	AA	937	A	N3-C4-C5	-9.72	119.99	126.80
26	BA	223	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	1253	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	2119	A	N3-C4-C5	-9.72	119.99	126.80
1	AA	466	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	535	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	1227	A	N3-C4-C5	-9.72	120.00	126.80
23	AW	14	A	N3-C4-C5	-9.72	120.00	126.80
23	AW	76	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	21	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	155	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	515	A	N3-C4-C5	-9.72	119.99	126.80
26	BA	497	A	N3-C4-C5	-9.72	120.00	126.80
27	BB	50	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	1447	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	742	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	126	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	526	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	752	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	1246	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	2126	A	N3-C4-C5	-9.72	120.00	126.80
27	BB	66	A	N3-C4-C5	-9.72	120.00	126.80
26	BA	1735	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	802	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1229	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1493	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	480	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	614	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	1757	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	1786	A	N3-C4-C5	-9.71	120.00	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2314	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	143	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	282	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	495	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	790	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	139	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	415	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	927	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	1133	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	2274	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	2482	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	459	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	1626	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	792	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1213	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1408	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	1413	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	1749	A	N3-C4-C5	-9.71	120.00	126.80
26	BA	1932	A	N3-C4-C5	-9.71	120.00	126.80
27	BB	45	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1256	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	2097	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	2278	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	2736	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	456	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	609	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	1257	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	213	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1205	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1286	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1304	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1794	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	2435	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	2534	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	2432	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	1500	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	2835	A	N3-C4-C5	-9.70	120.01	126.80
25	AY	73	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	104	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	127	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	221	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	788	A	N3-C4-C5	-9.70	120.01	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1073	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1284	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1739	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	2503	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	2682	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	718	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	1055	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	1130	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1586	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1616	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1690	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1918	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	263	A	N3-C4-C5	-9.69	120.01	126.80
1	AA	298	A	N3-C4-C5	-9.69	120.01	126.80
26	BA	227	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	1254	A	N3-C4-C5	-9.69	120.01	126.80
26	BA	1900	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	2020	A	N3-C4-C5	-9.69	120.01	126.80
26	BA	2376	A	N3-C4-C5	-9.70	120.01	126.80
26	BA	161	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	279	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	364	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	781	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	1689	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	374	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	819	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	1155	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	1614	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	2183	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	1394	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	1333	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	53	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	125	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	156	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	167	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	627	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	637	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	821	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	945	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	1322	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	1515	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	1654	A	N3-C4-C5	-9.69	120.02	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2147	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	2450	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	411	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	1081	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	89	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	936	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	51	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	815	A	N3-C4-C5	-9.69	120.02	126.80
23	AW	31	A	N3-C4-C5	-9.69	120.02	126.80
24	AX	9	A	N3-C4-C5	-9.69	120.02	126.80
26	BA	844	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	66	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	151	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	243	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	246	A	N3-C4-C5	-9.68	120.02	126.80
23	AW	51	A	N3-C4-C5	-9.68	120.02	126.80
26	BA	1080	A	N3-C4-C5	-9.68	120.02	126.80
26	BA	1551	A	N3-C4-C5	-9.68	120.02	126.80
26	BA	2031	A	N3-C4-C5	-9.68	120.02	126.80
26	BA	2059	A	N3-C4-C5	-9.68	120.02	126.80
26	BA	2614	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	80	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	250	A	N3-C4-C5	-9.68	120.02	126.80
26	BA	829	A	N3-C4-C5	-9.68	120.02	126.80
26	BA	1780	A	N3-C4-C5	-9.68	120.02	126.80
26	BA	1928	A	N3-C4-C5	-9.68	120.02	126.80
26	BA	1978	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	974	A	N3-C4-C5	-9.68	120.03	126.80
26	BA	2176	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	179	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	10	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	1000	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	1067	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	1117	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	1492	A	N3-C4-C5	-9.68	120.03	126.80
27	BB	46	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	77	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	502	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	547	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	1145	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	454	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	988	A	N3-C4-C5	-9.67	120.03	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1201	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	1275	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	1759	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	2590	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	1248	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	1289	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	63	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	73	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	91	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	2340	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	969	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	538	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	621	A	N3-C4-C5	-9.67	120.03	126.80
26	BA	2266	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	430	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	909	A	N3-C4-C5	-9.66	120.03	126.80
26	BA	477	A	N3-C4-C5	-9.66	120.03	126.80
26	BA	1713	A	N3-C4-C5	-9.66	120.03	126.80
26	BA	1854	A	N3-C4-C5	-9.66	120.03	126.80
27	BB	104	A	N3-C4-C5	-9.66	120.03	126.80
26	BA	782	A	N3-C4-C5	-9.66	120.04	126.80
26	BA	1593	A	N3-C4-C5	-9.66	120.04	126.80
26	BA	2513	A	N3-C4-C5	-9.66	120.04	126.80
26	BA	1129	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	315	A	N3-C4-C5	-9.66	120.04	126.80
26	BA	38	A	N3-C4-C5	-9.66	120.04	126.80
26	BA	483	A	N3-C4-C5	-9.66	120.04	126.80
26	BA	609	A	N3-C4-C5	-9.66	120.04	126.80
26	BA	1916	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	101	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	195	A	N3-C4-C5	-9.66	120.04	126.80
26	BA	1772	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	309	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	533	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	729	A	N3-C4-C5	-9.66	120.04	126.80
26	BA	2451	A	N3-C4-C5	-9.66	120.04	126.80
26	BA	340	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	196	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	493	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	520	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	759	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	1092	A	N3-C4-C5	-9.65	120.04	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1518	A	N3-C4-C5	-9.65	120.04	126.80
26	BA	603	A	N3-C4-C5	-9.65	120.04	126.80
26	BA	1700	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	321	A	N3-C4-C5	-9.65	120.04	126.80
26	BA	2298	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	602	A	N3-C4-C5	-9.65	120.05	126.80
26	BA	1808	A	N3-C4-C5	-9.65	120.05	126.80
26	BA	2679	A	N3-C4-C5	-9.65	120.04	126.80
26	BA	2734	A	N3-C4-C5	-9.65	120.04	126.80
26	BA	265	A	N3-C4-C5	-9.65	120.05	126.80
26	BA	920	A	N3-C4-C5	-9.65	120.05	126.80
26	BA	2388	A	N3-C4-C5	-9.65	120.05	126.80
25	AY	38	A	N3-C4-C5	-9.65	120.05	126.80
26	BA	2600	A	N3-C4-C5	-9.65	120.05	126.80
1	AA	182	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	507	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	2572	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	2598	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	1513	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	322	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	655	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	1134	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	2135	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	996	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	761	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	2542	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	1101	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	324	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	983	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	1420	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	2826	A	N3-C4-C5	-9.64	120.05	126.80
26	BA	1987	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	1246	A	N3-C4-C5	-9.64	120.06	126.80
26	BA	311	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	767	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	919	A	N3-C4-C5	-9.63	120.06	126.80
26	BA	2814	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	975	A	N3-C4-C5	-9.63	120.06	126.80
23	AW	66	A	N3-C4-C5	-9.63	120.06	126.80
26	BA	310	A	N3-C4-C5	-9.63	120.06	126.80
26	BA	1347	A	N3-C4-C5	-9.63	120.06	126.80
26	BA	1803	A	N3-C4-C5	-9.63	120.06	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1566	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	131	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	687	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	1250	A	N3-C4-C5	-9.63	120.06	126.80
26	BA	1057	A	N3-C4-C5	-9.63	120.06	126.80
26	BA	1285	A	N3-C4-C5	-9.63	120.06	126.80
26	BA	2726	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	50	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	1216	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	1285	A	N3-C4-C5	-9.63	120.06	126.80
26	BA	1677	A	N3-C4-C5	-9.62	120.06	126.80
1	AA	3	A	N3-C4-C5	-9.62	120.06	126.80
1	AA	238	A	N3-C4-C5	-9.62	120.06	126.80
1	AA	915	A	N3-C4-C5	-9.62	120.06	126.80
26	BA	1668	A	N3-C4-C5	-9.62	120.06	126.80
26	BA	1890	A	N3-C4-C5	-9.62	120.06	126.80
26	BA	783	A	N3-C4-C5	-9.62	120.06	126.80
1	AA	253	A	N3-C4-C5	-9.62	120.07	126.80
23	AW	42	A	N3-C4-C5	-9.62	120.07	126.80
26	BA	1705	A	N3-C4-C5	-9.62	120.07	126.80
26	BA	1204	A	N3-C4-C5	-9.62	120.07	126.80
26	BA	207	A	N3-C4-C5	-9.62	120.07	126.80
26	BA	1815	A	N3-C4-C5	-9.62	120.07	126.80
1	AA	44	A	N3-C4-C5	-9.61	120.07	126.80
26	BA	320	A	N3-C4-C5	-9.61	120.07	126.80
26	BA	1821	A	N3-C4-C5	-9.61	120.07	126.80
26	BA	2868	A	N3-C4-C5	-9.61	120.07	126.80
1	AA	766	A	N3-C4-C5	-9.61	120.07	126.80
26	BA	2448	A	N3-C4-C5	-9.61	120.07	126.80
26	BA	2829	A	N3-C4-C5	-9.61	120.07	126.80
1	AA	171	A	N3-C4-C5	-9.61	120.07	126.80
26	BA	1598	A	N3-C4-C5	-9.61	120.07	126.80
26	BA	2108	A	N3-C4-C5	-9.61	120.07	126.80
1	AA	197	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	338	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	681	A	N3-C4-C5	-9.60	120.08	126.80
27	BB	108	A	N3-C4-C5	-9.60	120.08	126.80
26	BA	973	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	327	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	1410	A	N3-C4-C5	-9.60	120.08	126.80
22	AV	15	A	N3-C4-C5	-9.60	120.08	126.80
22	AV	21	A	N3-C4-C5	-9.60	120.08	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2225	A	N3-C4-C5	-9.60	120.08	126.80
26	BA	2358	A	N3-C4-C5	-9.60	120.08	126.80
26	BA	676	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	554	A	N3-C4-C5	-9.60	120.08	126.80
26	BA	749	A	N3-C4-C5	-9.60	120.08	126.80
26	BA	1165	A	N3-C4-C5	-9.60	120.08	126.80
26	BA	1755	A	N3-C4-C5	-9.60	120.08	126.80
26	BA	947	A	N3-C4-C5	-9.59	120.08	126.80
26	BA	981	A	N3-C4-C5	-9.59	120.08	126.80
26	BA	1509	A	N3-C4-C5	-9.59	120.08	126.80
26	BA	1655	A	N3-C4-C5	-9.59	120.08	126.80
26	BA	1960	A	N3-C4-C5	-9.59	120.08	126.80
26	BA	2478	A	N3-C4-C5	-9.59	120.08	126.80
26	BA	2154	A	N3-C4-C5	-9.59	120.08	126.80
26	BA	2639	A	N3-C4-C5	-9.59	120.09	126.80
27	BB	58	A	N3-C4-C5	-9.59	120.08	126.80
1	AA	172	A	N3-C4-C5	-9.59	120.09	126.80
1	AA	665	A	N3-C4-C5	-9.59	120.09	126.80
26	BA	300	A	N3-C4-C5	-9.59	120.09	126.80
26	BA	1237	A	N3-C4-C5	-9.59	120.09	126.80
26	BA	2037	A	N3-C4-C5	-9.59	120.09	126.80
26	BA	990	A	N3-C4-C5	-9.59	120.09	126.80
1	AA	498	A	N3-C4-C5	-9.58	120.09	126.80
26	BA	586	A	N3-C4-C5	-9.58	120.09	126.80
26	BA	1265	A	N3-C4-C5	-9.58	120.09	126.80
26	BA	83	A	N3-C4-C5	-9.58	120.09	126.80
1	AA	349	A	N3-C4-C5	-9.58	120.09	126.80
1	AA	978	A	N3-C4-C5	-9.58	120.10	126.80
1	AA	1239	A	N3-C4-C5	-9.58	120.10	126.80
26	BA	1275	A	N3-C4-C5	-9.58	120.10	126.80
1	AA	878	A	N3-C4-C5	-9.57	120.10	126.80
26	BA	1652	A	N3-C4-C5	-9.57	120.10	126.80
26	BA	2741	A	N3-C4-C5	-9.57	120.10	126.80
26	BA	1077	A	N3-C4-C5	-9.57	120.10	126.80
26	BA	2418	A	N3-C4-C5	-9.57	120.10	126.80
26	BA	677	A	N3-C4-C5	-9.56	120.11	126.80
26	BA	1419	A	N3-C4-C5	-9.56	120.11	126.80
26	BA	2322	A	N3-C4-C5	-9.56	120.11	126.80
26	BA	1040	A	N3-C4-C5	-9.56	120.11	126.80
1	AA	1413	A	N3-C4-C5	-9.55	120.11	126.80
26	BA	529	A	N3-C4-C5	-9.55	120.11	126.80
26	BA	1032	A	N3-C4-C5	-9.55	120.11	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1590	A	N3-C4-C5	-9.55	120.11	126.80
26	BA	2247	A	N3-C4-C5	-9.55	120.11	126.80
1	AA	26	A	N3-C4-C5	-9.55	120.11	126.80
26	BA	84	A	N3-C4-C5	-9.55	120.11	126.80
26	BA	1001	A	N3-C4-C5	-9.55	120.11	126.80
26	BA	1913	A	N3-C4-C5	-9.55	120.11	126.80
1	AA	574	A	N3-C4-C5	-9.55	120.12	126.80
1	AA	412	A	N3-C4-C5	-9.54	120.12	126.80
26	BA	2566	A	N3-C4-C5	-9.54	120.12	126.80
26	BA	2090	A	N3-C4-C5	-9.54	120.12	126.80
26	BA	1937	A	N3-C4-C5	-9.54	120.12	126.80
26	BA	764	A	N3-C4-C5	-9.54	120.13	126.80
26	BA	1359	A	N3-C4-C5	-9.54	120.12	126.80
26	BA	241	A	N3-C4-C5	-9.53	120.13	126.80
1	AA	622	A	N3-C4-C5	-9.53	120.13	126.80
26	BA	2565	A	N3-C4-C5	-9.52	120.14	126.80
26	BA	1427	A	N3-C4-C5	-9.52	120.14	126.80
1	AA	16	A	N3-C4-C5	-9.52	120.14	126.80
26	BA	1522	A	N3-C4-C5	-9.51	120.14	126.80
1	AA	336	A	N3-C4-C5	-9.51	120.15	126.80
1	AA	1150	A	N3-C4-C5	-9.50	120.15	126.80
1	AA	60	A	N3-C4-C5	-9.49	120.15	126.80
1	AA	393	A	N3-C4-C5	-9.49	120.15	126.80
26	BA	1155	A	N3-C4-C5	-9.49	120.15	126.80
26	BA	2764	A	N3-C4-C5	-9.49	120.16	126.80
26	BA	2019	A	N3-C4-C5	-9.49	120.16	126.80
26	BA	2071	A	N3-C4-C5	-9.49	120.16	126.80
26	BA	905	A	N3-C4-C5	-9.48	120.16	126.80
26	BA	354	A	N3-C4-C5	-9.48	120.16	126.80
1	AA	913	A	N3-C4-C5	-9.48	120.16	126.80
26	BA	574	A	N3-C4-C5	-9.48	120.16	126.80
1	AA	1238	A	N3-C4-C5	-9.48	120.17	126.80
26	BA	2589	A	N3-C4-C5	-9.48	120.17	126.80
26	BA	1610	A	N3-C4-C5	-9.48	120.17	126.80
26	BA	42	A	N3-C4-C5	-9.47	120.17	126.80
26	BA	2009	A	N3-C4-C5	-9.47	120.17	126.80
26	BA	1545	A	N3-C4-C5	-9.47	120.17	126.80
26	BA	466	A	N3-C4-C5	-9.47	120.17	126.80
1	AA	1151	A	N3-C4-C5	-9.47	120.17	126.80
26	BA	1014	A	N3-C4-C5	-9.47	120.17	126.80
1	AA	1170	A	N3-C4-C5	-9.46	120.18	126.80
1	AA	1437	A	N3-C4-C5	-9.45	120.18	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1147	A	N3-C4-C5	-9.45	120.18	126.80
27	BB	34	A	N3-C4-C5	-9.45	120.19	126.80
1	AA	889	A	N3-C4-C5	-9.44	120.19	126.80
26	BA	2883	A	N3-C4-C5	-9.44	120.19	126.80
1	AA	74	A	N3-C4-C5	-9.44	120.19	126.80
26	BA	668	A	N3-C4-C5	-9.44	120.19	126.80
26	BA	1142	A	N3-C4-C5	-9.43	120.20	126.80
26	BA	2469	A	N3-C4-C5	-9.42	120.20	126.80
26	BA	1630	A	N3-C4-C5	-9.41	120.21	126.80
1	AA	452	A	N3-C4-C5	-9.40	120.22	126.80
26	BA	1785	A	N3-C4-C5	-9.39	120.23	126.80
26	BA	1953	A	N3-C4-C5	-9.37	120.24	126.80
26	BA	1378	A	N3-C4-C5	-9.36	120.25	126.80
26	BA	1385	A	N3-C4-C5	-9.34	120.26	126.80
26	BA	2033	A	N3-C4-C5	-9.34	120.27	126.80
26	BA	204	A	N3-C4-C5	-9.33	120.27	126.80
26	BA	119	A	N3-C4-C5	-9.31	120.28	126.80
26	BA	457	A	N3-C4-C5	-9.30	120.29	126.80
1	AA	1158	C	N1-C2-O2	9.27	124.46	118.90
26	BA	800	A	N3-C4-C5	-9.24	120.33	126.80
1	AA	499	A	N3-C4-C5	-9.17	120.38	126.80
1	AA	1329	A	N3-C4-C5	-9.15	120.40	126.80
26	BA	479	A	C5-N7-C8	9.14	108.47	103.90
1	AA	1158	C	C2-N1-C1'	8.90	128.59	118.80
1	AA	441	A	C5-N7-C8	8.63	108.21	103.90
26	BA	2776	A	C5-N7-C8	8.50	108.15	103.90
1	AA	1329	A	C5-N7-C8	8.49	108.14	103.90
26	BA	2070	A	C5-N7-C8	8.47	108.14	103.90
27	BB	52	A	C5-N7-C8	8.47	108.14	103.90
1	AA	499	A	C5-N7-C8	8.46	108.13	103.90
23	AW	41	A	C5-N7-C8	8.46	108.13	103.90
1	AA	694	A	C5-N7-C8	8.45	108.13	103.90
26	BA	371	A	C5-N7-C8	8.45	108.12	103.90
26	BA	1385	A	C5-N7-C8	8.44	108.12	103.90
26	BA	454	A	C5-N7-C8	8.43	108.12	103.90
1	AA	949	A	C5-N7-C8	8.42	108.11	103.90
1	AA	915	A	C5-N7-C8	8.42	108.11	103.90
1	AA	1368	A	C5-N7-C8	8.42	108.11	103.90
26	BA	819	A	C5-N7-C8	8.42	108.11	103.90
26	BA	2761	A	C5-N7-C8	8.41	108.11	103.90
1	AA	51	A	C5-N7-C8	8.41	108.11	103.90
26	BA	910	A	C5-N7-C8	8.40	108.10	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1937	A	C5-N7-C8	8.40	108.10	103.90
1	AA	414	A	C5-N7-C8	8.40	108.10	103.90
26	BA	2082	A	C5-N7-C8	8.40	108.10	103.90
1	AA	759	A	C5-N7-C8	8.39	108.10	103.90
1	AA	246	A	C5-N7-C8	8.39	108.10	103.90
24	AX	58	A	C5-N7-C8	8.39	108.10	103.90
1	AA	131	A	C5-N7-C8	8.39	108.09	103.90
26	BA	74	A	C5-N7-C8	8.39	108.09	103.90
26	BA	1634	A	C5-N7-C8	8.39	108.09	103.90
23	AW	51	A	C5-N7-C8	8.38	108.09	103.90
26	BA	2758	A	C5-N7-C8	8.39	108.09	103.90
26	BA	1773	A	C5-N7-C8	8.38	108.09	103.90
26	BA	1970	A	C5-N7-C8	8.38	108.09	103.90
26	BA	2418	A	C5-N7-C8	8.38	108.09	103.90
26	BA	191	A	C5-N7-C8	8.38	108.09	103.90
26	BA	2590	A	C5-N7-C8	8.37	108.09	103.90
1	AA	583	A	C5-N7-C8	8.37	108.09	103.90
1	AA	1418	A	C5-N7-C8	8.37	108.08	103.90
1	AA	8	A	C5-N7-C8	8.36	108.08	103.90
1	AA	243	A	C5-N7-C8	8.36	108.08	103.90
26	BA	2471	A	C5-N7-C8	8.36	108.08	103.90
26	BA	2322	A	C5-N7-C8	8.36	108.08	103.90
26	BA	2381	A	C5-N7-C8	8.36	108.08	103.90
1	AA	1374	A	C5-N7-C8	8.35	108.07	103.90
26	BA	1630	A	C5-N7-C8	8.35	108.07	103.90
26	BA	825	A	C5-N7-C8	8.35	108.07	103.90
26	BA	1597	A	C5-N7-C8	8.35	108.07	103.90
26	BA	471	A	C5-N7-C8	8.34	108.07	103.90
26	BA	1772	A	C5-N7-C8	8.34	108.07	103.90
26	BA	2589	A	C5-N7-C8	8.34	108.07	103.90
26	BA	1308	A	C5-N7-C8	8.34	108.07	103.90
26	BA	354	A	C5-N7-C8	8.33	108.07	103.90
26	BA	2101	A	C5-N7-C8	8.33	108.07	103.90
1	AA	649	A	C5-N7-C8	8.33	108.07	103.90
27	BB	34	A	C5-N7-C8	8.33	108.07	103.90
26	BA	1014	A	C5-N7-C8	8.33	108.06	103.90
1	AA	1311	A	C5-N7-C8	8.33	108.06	103.90
26	BA	1169	A	C5-N7-C8	8.33	108.06	103.90
26	BA	1304	A	C5-N7-C8	8.33	108.06	103.90
26	BA	1678	A	C5-N7-C8	8.32	108.06	103.90
1	AA	181	A	C5-N7-C8	8.32	108.06	103.90
1	AA	431	A	C5-N7-C8	8.32	108.06	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1155	A	C5-N7-C8	8.32	108.06	103.90
26	BA	693	A	C5-N7-C8	8.32	108.06	103.90
1	AA	19	A	C5-N7-C8	8.32	108.06	103.90
1	AA	465	A	C5-N7-C8	8.32	108.06	103.90
26	BA	2241	A	C5-N7-C8	8.32	108.06	103.90
1	AA	44	A	C5-N7-C8	8.32	108.06	103.90
1	AA	554	A	C5-N7-C8	8.32	108.06	103.90
26	BA	2657	A	C5-N7-C8	8.32	108.06	103.90
1	AA	1105	A	C5-N7-C8	8.32	108.06	103.90
23	AW	14	A	C5-N7-C8	8.32	108.06	103.90
26	BA	231	A	C5-N7-C8	8.32	108.06	103.90
26	BA	1609	A	C5-N7-C8	8.32	108.06	103.90
26	BA	1969	A	C5-N7-C8	8.31	108.06	103.90
1	AA	435	A	C5-N7-C8	8.31	108.06	103.90
1	AA	681	A	C5-N7-C8	8.31	108.06	103.90
26	BA	265	A	C5-N7-C8	8.31	108.06	103.90
23	AW	26	A	C5-N7-C8	8.31	108.05	103.90
26	BA	1746	A	C5-N7-C8	8.31	108.05	103.90
26	BA	2388	A	C5-N7-C8	8.30	108.05	103.90
1	AA	749	A	C5-N7-C8	8.30	108.05	103.90
1	AA	1483	A	C5-N7-C8	8.30	108.05	103.90
26	BA	38	A	C5-N7-C8	8.30	108.05	103.90
26	BA	1553	A	C5-N7-C8	8.30	108.05	103.90
26	BA	2778	A	C5-N7-C8	8.30	108.05	103.90
1	AA	1055	A	C5-N7-C8	8.30	108.05	103.90
26	BA	1054	A	C5-N7-C8	8.30	108.05	103.90
26	BA	1089	A	C5-N7-C8	8.30	108.05	103.90
1	AA	753	A	C5-N7-C8	8.29	108.05	103.90
1	AA	1146	A	C5-N7-C8	8.29	108.05	103.90
26	BA	480	A	C5-N7-C8	8.29	108.05	103.90
26	BA	800	A	C5-N7-C8	8.29	108.05	103.90
26	BA	1165	A	C5-N7-C8	8.29	108.05	103.90
26	BA	1175	A	C5-N7-C8	8.29	108.05	103.90
1	AA	55	A	C5-N7-C8	8.29	108.05	103.90
1	AA	602	A	C5-N7-C8	8.29	108.05	103.90
1	AA	695	A	C5-N7-C8	8.29	108.05	103.90
26	BA	5	A	C5-N7-C8	8.29	108.05	103.90
26	BA	1494	A	C5-N7-C8	8.29	108.05	103.90
26	BA	155	A	C5-N7-C8	8.29	108.05	103.90
26	BA	2542	A	C5-N7-C8	8.29	108.05	103.90
1	AA	223	A	C5-N7-C8	8.29	108.04	103.90
1	AA	363	A	C5-N7-C8	8.29	108.04	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1248	A	C5-N7-C8	8.29	108.04	103.90
26	BA	861	A	C5-N7-C8	8.29	108.04	103.90
26	BA	165	A	C5-N7-C8	8.29	108.04	103.90
1	AA	825	A	C5-N7-C8	8.28	108.04	103.90
1	AA	860	A	C5-N7-C8	8.28	108.04	103.90
26	BA	538	A	C5-N7-C8	8.28	108.04	103.90
26	BA	1029	A	C5-N7-C8	8.28	108.04	103.90
26	BA	541	A	C5-N7-C8	8.28	108.04	103.90
26	BA	917	A	C5-N7-C8	8.28	108.04	103.90
26	BA	1147	A	C5-N7-C8	8.28	108.04	103.90
26	BA	1913	A	C5-N7-C8	8.28	108.04	103.90
1	AA	199	A	C5-N7-C8	8.28	108.04	103.90
1	AA	1492	A	C5-N7-C8	8.28	108.04	103.90
1	AA	1503	A	C5-N7-C8	8.28	108.04	103.90
26	BA	149	A	C5-N7-C8	8.28	108.04	103.90
26	BA	829	A	C5-N7-C8	8.28	108.04	103.90
26	BA	256	A	C5-N7-C8	8.28	108.04	103.90
26	BA	470	A	C5-N7-C8	8.28	108.04	103.90
26	BA	2281	A	C5-N7-C8	8.28	108.04	103.90
26	BA	2352	A	C5-N7-C8	8.28	108.04	103.90
1	AA	320	A	C5-N7-C8	8.27	108.04	103.90
26	BA	1717	A	C5-N7-C8	8.27	108.04	103.90
26	BA	2003	A	C5-N7-C8	8.27	108.04	103.90
26	BA	2377	A	C5-N7-C8	8.27	108.04	103.90
26	BA	2534	A	C5-N7-C8	8.27	108.04	103.90
26	BA	2665	A	C5-N7-C8	8.27	108.04	103.90
1	AA	129	A	C5-N7-C8	8.27	108.04	103.90
1	AA	794	A	C5-N7-C8	8.27	108.03	103.90
1	AA	918	A	C5-N7-C8	8.27	108.03	103.90
26	BA	1641	A	C5-N7-C8	8.27	108.04	103.90
26	BA	2335	A	C5-N7-C8	8.27	108.04	103.90
26	BA	2406	A	C5-N7-C8	8.27	108.04	103.90
26	BA	1590	A	C5-N7-C8	8.27	108.03	103.90
26	BA	2033	A	C5-N7-C8	8.27	108.03	103.90
1	AA	635	A	C5-N7-C8	8.27	108.03	103.90
23	AW	42	A	C5-N7-C8	8.27	108.03	103.90
26	BA	1143	A	C5-N7-C8	8.27	108.03	103.90
26	BA	1230	A	C5-N7-C8	8.27	108.03	103.90
26	BA	1722	A	C5-N7-C8	8.27	108.03	103.90
26	BA	49	A	C5-N7-C8	8.27	108.03	103.90
26	BA	1794	A	C5-N7-C8	8.27	108.03	103.90
1	AA	152	A	C5-N7-C8	8.27	108.03	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	332	A	C5-N7-C8	8.27	108.03	103.90
1	AA	1176	A	C5-N7-C8	8.26	108.03	103.90
26	BA	1213	A	C5-N7-C8	8.26	108.03	103.90
26	BA	1655	A	C5-N7-C8	8.26	108.03	103.90
26	BA	1354	A	C5-N7-C8	8.26	108.03	103.90
26	BA	1509	A	C5-N7-C8	8.26	108.03	103.90
26	BA	1916	A	C5-N7-C8	8.26	108.03	103.90
26	BA	2726	A	C5-N7-C8	8.26	108.03	103.90
1	AA	10	A	C5-N7-C8	8.26	108.03	103.90
26	BA	382	A	C5-N7-C8	8.26	108.03	103.90
26	BA	1749	A	C5-N7-C8	8.26	108.03	103.90
1	AA	907	A	C5-N7-C8	8.26	108.03	103.90
1	AA	1493	A	C5-N7-C8	8.26	108.03	103.90
26	BA	320	A	C5-N7-C8	8.26	108.03	103.90
26	BA	1040	A	C5-N7-C8	8.26	108.03	103.90
26	BA	2134	A	C5-N7-C8	8.26	108.03	103.90
1	AA	1102	A	C5-N7-C8	8.26	108.03	103.90
1	AA	1151	A	C5-N7-C8	8.26	108.03	103.90
1	AA	1299	A	C5-N7-C8	8.26	108.03	103.90
26	BA	599	A	C5-N7-C8	8.26	108.03	103.90
26	BA	996	A	C5-N7-C8	8.26	108.03	103.90
26	BA	2814	A	C5-N7-C8	8.26	108.03	103.90
1	AA	802	A	C5-N7-C8	8.26	108.03	103.90
23	AW	58	A	C5-N7-C8	8.26	108.03	103.90
26	BA	2634	A	C5-N7-C8	8.26	108.03	103.90
1	AA	466	A	C5-N7-C8	8.25	108.03	103.90
1	AA	1398	A	C5-N7-C8	8.25	108.03	103.90
26	BA	223	A	C5-N7-C8	8.25	108.03	103.90
26	BA	1848	A	C5-N7-C8	8.25	108.03	103.90
26	BA	1960	A	C5-N7-C8	8.25	108.03	103.90
26	BA	84	A	C5-N7-C8	8.25	108.03	103.90
26	BA	131	A	C5-N7-C8	8.25	108.03	103.90
26	BA	2147	A	C5-N7-C8	8.25	108.03	103.90
26	BA	2288	A	C5-N7-C8	8.25	108.03	103.90
26	BA	2736	A	C5-N7-C8	8.25	108.03	103.90
26	BA	2829	A	C5-N7-C8	8.25	108.03	103.90
1	AA	1408	A	C5-N7-C8	8.25	108.02	103.90
22	AV	22	A	C5-N7-C8	8.25	108.03	103.90
26	BA	176	A	C5-N7-C8	8.25	108.03	103.90
26	BA	1755	A	C5-N7-C8	8.25	108.02	103.90
26	BA	1966	A	C5-N7-C8	8.25	108.03	103.90
26	BA	2126	A	C5-N7-C8	8.25	108.02	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	253	A	C5-N7-C8	8.25	108.02	103.90
1	AA	329	A	C5-N7-C8	8.25	108.02	103.90
1	AA	1000	A	C5-N7-C8	8.25	108.02	103.90
26	BA	111	A	C5-N7-C8	8.25	108.02	103.90
26	BA	502	A	C5-N7-C8	8.25	108.02	103.90
26	BA	739	A	C5-N7-C8	8.25	108.02	103.90
26	BA	1569	A	C5-N7-C8	8.25	108.02	103.90
26	BA	2882	A	C5-N7-C8	8.25	108.02	103.90
26	BA	2183	A	C5-N7-C8	8.24	108.02	103.90
1	AA	155	A	C5-N7-C8	8.24	108.02	103.90
1	AA	1019	A	C5-N7-C8	8.24	108.02	103.90
26	BA	453	A	C5-N7-C8	8.24	108.02	103.90
26	BA	1287	A	C5-N7-C8	8.24	108.02	103.90
26	BA	1938	A	C5-N7-C8	8.24	108.02	103.90
1	AA	179	A	C5-N7-C8	8.24	108.02	103.90
26	BA	2314	A	C5-N7-C8	8.24	108.02	103.90
1	AA	371	A	C5-N7-C8	8.24	108.02	103.90
1	AA	815	A	C5-N7-C8	8.24	108.02	103.90
26	BA	905	A	C5-N7-C8	8.24	108.02	103.90
26	BA	1700	A	C5-N7-C8	8.24	108.02	103.90
26	BA	1420	A	C5-N7-C8	8.24	108.02	103.90
26	BA	2270	A	C5-N7-C8	8.24	108.02	103.90
1	AA	300	A	C5-N7-C8	8.24	108.02	103.90
1	AA	349	A	C5-N7-C8	8.24	108.02	103.90
1	AA	383	A	C5-N7-C8	8.24	108.02	103.90
1	AA	1349	A	C5-N7-C8	8.24	108.02	103.90
26	BA	402	A	C5-N7-C8	8.24	108.02	103.90
26	BA	505	A	C5-N7-C8	8.24	108.02	103.90
26	BA	621	A	C5-N7-C8	8.24	108.02	103.90
26	BA	718	A	C5-N7-C8	8.24	108.02	103.90
26	BA	849	A	C5-N7-C8	8.24	108.02	103.90
26	BA	927	A	C5-N7-C8	8.24	108.02	103.90
1	AA	373	A	C5-N7-C8	8.23	108.02	103.90
1	AA	50	A	C5-N7-C8	8.23	108.02	103.90
1	AA	673	A	C5-N7-C8	8.23	108.02	103.90
1	AA	696	A	C5-N7-C8	8.23	108.02	103.90
1	AA	978	A	C5-N7-C8	8.23	108.02	103.90
1	AA	1204	A	C5-N7-C8	8.23	108.02	103.90
1	AA	1410	A	C5-N7-C8	8.23	108.02	103.90
26	BA	432	A	C5-N7-C8	8.23	108.02	103.90
26	BA	1237	A	C5-N7-C8	8.23	108.02	103.90
26	BA	1502	A	C5-N7-C8	8.23	108.02	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1919	A	C5-N7-C8	8.23	108.02	103.90
26	BA	2117	A	C5-N7-C8	8.23	108.02	103.90
26	BA	2435	A	C5-N7-C8	8.23	108.02	103.90
26	BA	1571	A	C5-N7-C8	8.23	108.02	103.90
27	BB	109	A	C5-N7-C8	8.23	108.02	103.90
1	AA	78	A	C5-N7-C8	8.23	108.02	103.90
1	AA	461	A	C5-N7-C8	8.23	108.02	103.90
1	AA	1257	A	C5-N7-C8	8.23	108.02	103.90
26	BA	603	A	C5-N7-C8	8.23	108.02	103.90
26	BA	1050	A	C5-N7-C8	8.23	108.02	103.90
26	BA	1551	A	C5-N7-C8	8.23	108.02	103.90
26	BA	2142	A	C5-N7-C8	8.23	108.02	103.90
26	BA	1786	A	C5-N7-C8	8.23	108.01	103.90
1	AA	210	C	N1-C2-O2	8.23	123.84	118.90
26	BA	95	A	C5-N7-C8	8.23	108.01	103.90
26	BA	270	A	C5-N7-C8	8.23	108.02	103.90
26	BA	401	A	C5-N7-C8	8.23	108.01	103.90
26	BA	1272	A	C5-N7-C8	8.23	108.02	103.90
26	BA	2060	A	C5-N7-C8	8.23	108.01	103.90
26	BA	2461	A	C5-N7-C8	8.23	108.01	103.90
26	BA	160	A	C5-N7-C8	8.23	108.01	103.90
26	BA	706	A	C5-N7-C8	8.23	108.01	103.90
26	BA	1998	A	C5-N7-C8	8.23	108.01	103.90
1	AA	411	A	C5-N7-C8	8.22	108.01	103.90
1	AA	648	A	C5-N7-C8	8.22	108.01	103.90
1	AA	1179	A	C5-N7-C8	8.22	108.01	103.90
23	AW	23	A	C5-N7-C8	8.22	108.01	103.90
26	BA	42	A	C5-N7-C8	8.22	108.01	103.90
26	BA	204	A	C5-N7-C8	8.22	108.01	103.90
26	BA	217	A	C5-N7-C8	8.22	108.01	103.90
26	BA	1987	A	C5-N7-C8	8.22	108.01	103.90
1	AA	913	A	C5-N7-C8	8.22	108.01	103.90
26	BA	449	A	C5-N7-C8	8.22	108.01	103.90
26	BA	492	A	C5-N7-C8	8.22	108.01	103.90
26	BA	2518	A	C5-N7-C8	8.22	108.01	103.90
26	BA	457	A	C5-N7-C8	8.22	108.01	103.90
26	BA	2268	A	C5-N7-C8	8.22	108.01	103.90
26	BA	2566	A	C5-N7-C8	8.22	108.01	103.90
1	AA	1225	A	C5-N7-C8	8.22	108.01	103.90
1	AA	1280	A	C5-N7-C8	8.22	108.01	103.90
1	AA	1428	A	C5-N7-C8	8.22	108.01	103.90
26	BA	182	A	C5-N7-C8	8.22	108.01	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	352	A	C5-N7-C8	8.22	108.01	103.90
26	BA	802	A	C5-N7-C8	8.22	108.01	103.90
26	BA	1698	A	C5-N7-C8	8.22	108.01	103.90
26	BA	2009	A	C5-N7-C8	8.22	108.01	103.90
26	BA	2513	A	C5-N7-C8	8.22	108.01	103.90
26	BA	2600	A	C5-N7-C8	8.22	108.01	103.90
26	BA	2748	A	C5-N7-C8	8.22	108.01	103.90
26	BA	2019	A	C5-N7-C8	8.22	108.01	103.90
26	BA	2176	A	C5-N7-C8	8.22	108.01	103.90
1	AA	120	A	C5-N7-C8	8.21	108.01	103.90
26	BA	2851	A	C5-N7-C8	8.22	108.01	103.90
1	AA	288	A	C5-N7-C8	8.21	108.01	103.90
1	AA	706	A	C5-N7-C8	8.21	108.01	103.90
1	AA	767	A	C5-N7-C8	8.21	108.01	103.90
1	AA	1246	A	C5-N7-C8	8.21	108.01	103.90
24	AX	26	A	C5-N7-C8	8.21	108.01	103.90
26	BA	28	A	C5-N7-C8	8.22	108.01	103.90
26	BA	513	A	C5-N7-C8	8.22	108.01	103.90
26	BA	1871	A	C5-N7-C8	8.22	108.01	103.90
26	BA	172	A	C5-N7-C8	8.21	108.01	103.90
26	BA	1268	A	C5-N7-C8	8.21	108.01	103.90
26	BA	1650	A	C5-N7-C8	8.21	108.01	103.90
26	BA	2516	A	C5-N7-C8	8.21	108.01	103.90
1	AA	210	C	C2-N1-C1'	8.21	127.83	118.80
1	AA	640	A	C5-N7-C8	8.21	108.01	103.90
1	AA	946	A	C5-N7-C8	8.21	108.01	103.90
1	AA	1196	A	C5-N7-C8	8.21	108.01	103.90
1	AA	1502	A	C5-N7-C8	8.21	108.01	103.90
24	AX	9	A	C5-N7-C8	8.21	108.01	103.90
26	BA	101	A	C5-N7-C8	8.21	108.01	103.90
26	BA	190	A	C5-N7-C8	8.21	108.01	103.90
26	BA	878	A	C5-N7-C8	8.21	108.01	103.90
26	BA	1142	A	C5-N7-C8	8.21	108.01	103.90
26	BA	1367	A	C5-N7-C8	8.21	108.01	103.90
26	BA	2309	A	C5-N7-C8	8.21	108.01	103.90
26	BA	1069	A	C5-N7-C8	8.21	108.00	103.90
26	BA	1366	A	C5-N7-C8	8.21	108.00	103.90
26	BA	1652	A	C5-N7-C8	8.21	108.00	103.90
26	BA	2899	A	C5-N7-C8	8.21	108.00	103.90
1	AA	892	A	C5-N7-C8	8.21	108.00	103.90
1	AA	908	A	C5-N7-C8	8.21	108.00	103.90
1	AA	974	A	C5-N7-C8	8.21	108.00	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	788	A	C5-N7-C8	8.21	108.00	103.90
26	BA	1008	A	C5-N7-C8	8.21	108.00	103.90
26	BA	1032	A	C5-N7-C8	8.21	108.00	103.90
26	BA	1057	A	C5-N7-C8	8.21	108.00	103.90
26	BA	2530	A	C5-N7-C8	8.21	108.00	103.90
27	BB	108	A	C5-N7-C8	8.21	108.00	103.90
1	AA	309	A	C5-N7-C8	8.21	108.00	103.90
1	AA	366	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1111	A	C5-N7-C8	8.21	108.00	103.90
1	AA	1150	A	C5-N7-C8	8.21	108.00	103.90
1	AA	1468	A	C5-N7-C8	8.21	108.00	103.90
26	BA	2727	A	C5-N7-C8	8.21	108.00	103.90
26	BA	2740	A	C5-N7-C8	8.21	108.00	103.90
1	AA	1377	A	C5-N7-C8	8.20	108.00	103.90
26	BA	804	A	C5-N7-C8	8.20	108.00	103.90
26	BA	1952	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2632	A	C5-N7-C8	8.21	108.00	103.90
26	BA	2821	A	C5-N7-C8	8.20	108.00	103.90
1	AA	878	A	C5-N7-C8	8.20	108.00	103.90
23	AW	21	A	C5-N7-C8	8.20	108.00	103.90
26	BA	103	A	C5-N7-C8	8.20	108.00	103.90
26	BA	195	A	C5-N7-C8	8.20	108.00	103.90
26	BA	310	A	C5-N7-C8	8.20	108.00	103.90
26	BA	936	A	C5-N7-C8	8.20	108.00	103.90
26	BA	344	A	C5-N7-C8	8.20	108.00	103.90
26	BA	482	A	C5-N7-C8	8.20	108.00	103.90
26	BA	1189	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2014	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2900	A	C5-N7-C8	8.20	108.00	103.90
1	AA	74	A	C5-N7-C8	8.20	108.00	103.90
1	AA	432	A	C5-N7-C8	8.20	108.00	103.90
1	AA	655	A	C5-N7-C8	8.20	108.00	103.90
1	AA	782	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1476	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1012	A	C5-N7-C8	8.20	108.00	103.90
26	BA	483	A	C5-N7-C8	8.20	108.00	103.90
26	BA	547	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2411	A	C5-N7-C8	8.20	108.00	103.90
1	AA	167	A	C5-N7-C8	8.20	108.00	103.90
1	AA	448	A	C5-N7-C8	8.20	108.00	103.90
1	AA	553	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1250	A	C5-N7-C8	8.20	108.00	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	14	A	C5-N7-C8	8.20	108.00	103.90
26	BA	19	A	C5-N7-C8	8.20	108.00	103.90
26	BA	216	A	C5-N7-C8	8.20	108.00	103.90
26	BA	374	A	C5-N7-C8	8.20	108.00	103.90
26	BA	655	A	C5-N7-C8	8.20	108.00	103.90
26	BA	899	A	C5-N7-C8	8.20	108.00	103.90
26	BA	1126	A	C5-N7-C8	8.20	108.00	103.90
26	BA	1194	A	C5-N7-C8	8.20	108.00	103.90
26	BA	1205	A	C5-N7-C8	8.20	108.00	103.90
26	BA	1254	A	C5-N7-C8	8.20	108.00	103.90
26	BA	1353	A	C5-N7-C8	8.20	108.00	103.90
26	BA	1503	A	C5-N7-C8	8.20	108.00	103.90
26	BA	1918	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2154	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2211	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2426	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1213	A	C5-N7-C8	8.19	108.00	103.90
26	BA	255	A	C5-N7-C8	8.19	108.00	103.90
26	BA	2346	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2560	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2705	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2753	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2873	A	C5-N7-C8	8.20	108.00	103.90
26	BA	2850	A	C5-N7-C8	8.19	108.00	103.90
27	BB	53	A	C5-N7-C8	8.20	108.00	103.90
1	AA	109	A	C5-N7-C8	8.19	108.00	103.90
1	AA	130	A	C5-N7-C8	8.19	108.00	103.90
25	AY	38	A	C5-N7-C8	8.19	108.00	103.90
1	AA	968	A	C5-N7-C8	8.19	108.00	103.90
26	BA	6	A	C5-N7-C8	8.19	108.00	103.90
26	BA	1821	A	C5-N7-C8	8.19	108.00	103.90
26	BA	1853	A	C5-N7-C8	8.19	108.00	103.90
26	BA	2700	A	C5-N7-C8	8.19	108.00	103.90
26	BA	2738	A	C5-N7-C8	8.19	108.00	103.90
27	BB	15	A	C5-N7-C8	8.19	108.00	103.90
27	BB	59	A	C5-N7-C8	8.19	108.00	103.90
1	AA	98	A	C5-N7-C8	8.19	108.00	103.90
1	AA	325	A	C5-N7-C8	8.19	108.00	103.90
1	AA	1042	A	C5-N7-C8	8.19	108.00	103.90
25	AY	26	A	C5-N7-C8	8.19	108.00	103.90
26	BA	666	A	C5-N7-C8	8.19	108.00	103.90
26	BA	705	A	C5-N7-C8	8.19	108.00	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	508	A	C5-N7-C8	8.19	107.99	103.90
26	BA	1247	A	C5-N7-C8	8.19	107.99	103.90
26	BA	1427	A	C5-N7-C8	8.19	107.99	103.90
1	AA	65	A	C5-N7-C8	8.19	107.99	103.90
1	AA	72	A	C5-N7-C8	8.19	107.99	103.90
1	AA	456	A	C5-N7-C8	8.19	107.99	103.90
26	BA	699	A	C5-N7-C8	8.19	107.99	103.90
26	BA	945	A	C5-N7-C8	8.19	107.99	103.90
1	AA	1117	A	C5-N7-C8	8.19	107.99	103.90
1	AA	1287	A	C5-N7-C8	8.19	107.99	103.90
25	AY	14	A	C5-N7-C8	8.19	107.99	103.90
26	BA	1103	A	C5-N7-C8	8.19	107.99	103.90
26	BA	1809	A	C5-N7-C8	8.19	107.99	103.90
26	BA	1847	A	C5-N7-C8	8.19	107.99	103.90
26	BA	2077	A	C5-N7-C8	8.19	107.99	103.90
26	BA	2721	A	C5-N7-C8	8.19	107.99	103.90
1	AA	139	A	C5-N7-C8	8.18	107.99	103.90
1	AA	629	A	C5-N7-C8	8.18	107.99	103.90
1	AA	994	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1339	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1500	A	C5-N7-C8	8.18	107.99	103.90
25	AY	35	A	C5-N7-C8	8.18	107.99	103.90
26	BA	979	A	C5-N7-C8	8.18	107.99	103.90
26	BA	1593	A	C5-N7-C8	8.18	107.99	103.90
26	BA	2173	A	C5-N7-C8	8.18	107.99	103.90
26	BA	2572	A	C5-N7-C8	8.18	107.99	103.90
26	BA	507	A	C5-N7-C8	8.18	107.99	103.90
26	BA	2198	A	C5-N7-C8	8.18	107.99	103.90
26	BA	2311	A	C5-N7-C8	8.18	107.99	103.90
26	BA	2503	A	C5-N7-C8	8.18	107.99	103.90
1	AA	630	A	C5-N7-C8	8.18	107.99	103.90
1	AA	873	A	C5-N7-C8	8.18	107.99	103.90
1	AA	900	A	C5-N7-C8	8.18	107.99	103.90
1	AA	937	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1318	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1360	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1499	A	C5-N7-C8	8.18	107.99	103.90
26	BA	71	A	C5-N7-C8	8.18	107.99	103.90
26	BA	959	A	C5-N7-C8	8.18	107.99	103.90
26	BA	1877	A	C5-N7-C8	8.18	107.99	103.90
26	BA	2577	A	C5-N7-C8	8.18	107.99	103.90
1	AA	7	A	C5-N7-C8	8.18	107.99	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1394	A	C5-N7-C8	8.18	107.99	103.90
26	BA	299	A	C5-N7-C8	8.18	107.99	103.90
26	BA	608	A	C5-N7-C8	8.18	107.99	103.90
26	BA	2031	A	C5-N7-C8	8.18	107.99	103.90
26	BA	2602	A	C5-N7-C8	8.18	107.99	103.90
27	BB	58	A	C5-N7-C8	8.18	107.99	103.90
1	AA	80	A	C5-N7-C8	8.18	107.99	103.90
1	AA	162	A	C5-N7-C8	8.18	107.99	103.90
1	AA	938	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1518	A	C5-N7-C8	8.18	107.99	103.90
23	AW	69	A	C5-N7-C8	8.18	107.99	103.90
26	BA	125	A	C5-N7-C8	8.18	107.99	103.90
26	BA	340	A	C5-N7-C8	8.18	107.99	103.90
26	BA	348	A	C5-N7-C8	8.18	107.99	103.90
26	BA	1085	A	C5-N7-C8	8.18	107.99	103.90
26	BA	1801	A	C5-N7-C8	8.18	107.99	103.90
1	AA	535	A	C5-N7-C8	8.18	107.99	103.90
23	AW	59	A	C5-N7-C8	8.18	107.99	103.90
26	BA	347	A	C5-N7-C8	8.18	107.99	103.90
26	BA	1134	A	C5-N7-C8	8.18	107.99	103.90
26	BA	1739	A	C5-N7-C8	8.18	107.99	103.90
26	BA	1808	A	C5-N7-C8	8.18	107.99	103.90
26	BA	2750	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1413	A	C5-N7-C8	8.17	107.99	103.90
26	BA	241	A	C5-N7-C8	8.17	107.99	103.90
26	BA	477	A	C5-N7-C8	8.17	107.99	103.90
26	BA	609	A	C5-N7-C8	8.17	107.99	103.90
26	BA	794	A	C5-N7-C8	8.17	107.99	103.90
26	BA	1144	A	C5-N7-C8	8.17	107.99	103.90
26	BA	2090	A	C5-N7-C8	8.17	107.99	103.90
26	BA	1127	A	C5-N7-C8	8.17	107.99	103.90
26	BA	1307	A	C5-N7-C8	8.17	107.99	103.90
26	BA	2284	A	C5-N7-C8	8.17	107.99	103.90
26	BA	2893	A	C5-N7-C8	8.17	107.99	103.90
1	AA	53	A	C5-N7-C8	8.17	107.98	103.90
1	AA	1251	A	C5-N7-C8	8.17	107.99	103.90
26	BA	439	A	C5-N7-C8	8.17	107.98	103.90
1	AA	60	A	C5-N7-C8	8.17	107.98	103.90
1	AA	151	A	C5-N7-C8	8.17	107.98	103.90
1	AA	663	A	C5-N7-C8	8.17	107.98	103.90
1	AA	676	A	C5-N7-C8	8.17	107.98	103.90
1	AA	792	A	C5-N7-C8	8.17	107.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1239	A	C5-N7-C8	8.17	107.98	103.90
23	AW	38	A	C5-N7-C8	8.17	107.98	103.90
24	AX	41	A	C5-N7-C8	8.17	107.99	103.90
26	BA	918	A	C5-N7-C8	8.17	107.98	103.90
26	BA	2765	A	C5-N7-C8	8.17	107.98	103.90
26	BA	1637	A	C5-N7-C8	8.17	107.98	103.90
26	BA	2682	A	C5-N7-C8	8.17	107.98	103.90
1	AA	197	A	C5-N7-C8	8.17	107.98	103.90
26	BA	2013	A	C5-N7-C8	8.17	107.98	103.90
1	AA	274	A	C5-N7-C8	8.17	107.98	103.90
1	AA	573	A	C5-N7-C8	8.17	107.98	103.90
26	BA	391	A	C5-N7-C8	8.17	107.98	103.90
26	BA	428	A	C5-N7-C8	8.17	107.98	103.90
26	BA	2734	A	C5-N7-C8	8.17	107.98	103.90
26	BA	460	A	C5-N7-C8	8.17	107.98	103.90
27	BB	29	A	C5-N7-C8	8.17	107.98	103.90
1	AA	716	A	C5-N7-C8	8.16	107.98	103.90
1	AA	747	A	C5-N7-C8	8.16	107.98	103.90
1	AA	718	A	C5-N7-C8	8.16	107.98	103.90
1	AA	831	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1433	A	C5-N7-C8	8.16	107.98	103.90
24	AX	21	A	C5-N7-C8	8.16	107.98	103.90
25	AY	6	A	C5-N7-C8	8.16	107.98	103.90
25	AY	23	A	C5-N7-C8	8.16	107.98	103.90
26	BA	144	A	C5-N7-C8	8.16	107.98	103.90
26	BA	152	A	C5-N7-C8	8.16	107.98	103.90
26	BA	181	A	C5-N7-C8	8.16	107.98	103.90
26	BA	781	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1046	A	C5-N7-C8	8.16	107.98	103.90
26	BA	2170	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1429	A	C5-N7-C8	8.16	107.98	103.90
26	BA	556	A	C5-N7-C8	8.16	107.98	103.90
26	BA	602	A	C5-N7-C8	8.16	107.98	103.90
26	BA	742	A	C5-N7-C8	8.16	107.98	103.90
26	BA	792	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1070	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1336	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1431	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1080	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1572	A	C5-N7-C8	8.16	107.98	103.90
26	BA	2108	A	C5-N7-C8	8.16	107.98	103.90
26	BA	2433	A	C5-N7-C8	8.16	107.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	228	A	C5-N7-C8	8.16	107.98	103.90
1	AA	460	A	C5-N7-C8	8.16	107.98	103.90
1	AA	687	A	C5-N7-C8	8.16	107.98	103.90
1	AA	781	A	C5-N7-C8	8.16	107.98	103.90
26	BA	526	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1532	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1340	A	C5-N7-C8	8.16	107.98	103.90
26	BA	197	A	C5-N7-C8	8.16	107.98	103.90
26	BA	644	A	C5-N7-C8	8.16	107.98	103.90
26	BA	900	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1640	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1654	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1757	A	C5-N7-C8	8.16	107.98	103.90
26	BA	2358	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1535	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1544	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1552	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1566	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1805	A	C5-N7-C8	8.16	107.98	103.90
26	BA	2482	A	C5-N7-C8	8.16	107.98	103.90
26	BA	89	A	C5-N7-C8	8.16	107.98	103.90
26	BA	345	A	C5-N7-C8	8.16	107.98	103.90
26	BA	614	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1111	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1705	A	C5-N7-C8	8.16	107.98	103.90
26	BA	2247	A	C5-N7-C8	8.16	107.98	103.90
1	AA	621	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1229	A	C5-N7-C8	8.16	107.98	103.90
26	BA	64	A	C5-N7-C8	8.16	107.98	103.90
26	BA	126	A	C5-N7-C8	8.16	107.98	103.90
26	BA	222	A	C5-N7-C8	8.16	107.98	103.90
26	BA	501	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1508	A	C5-N7-C8	8.16	107.98	103.90
26	BA	1754	A	C5-N7-C8	8.16	107.98	103.90
26	BA	2298	A	C5-N7-C8	8.16	107.98	103.90
27	BB	119	A	C5-N7-C8	8.16	107.98	103.90
26	BA	2476	A	C5-N7-C8	8.16	107.98	103.90
26	BA	877	A	C5-N7-C8	8.15	107.98	103.90
26	BA	1048	A	C5-N7-C8	8.15	107.98	103.90
1	AA	59	A	C5-N7-C8	8.15	107.98	103.90
1	AA	189	A	C5-N7-C8	8.15	107.98	103.90
1	AA	572	A	C5-N7-C8	8.15	107.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	743	A	C5-N7-C8	8.15	107.98	103.90
1	AA	807	A	C5-N7-C8	8.15	107.98	103.90
1	AA	1197	A	C5-N7-C8	8.15	107.98	103.90
1	AA	1236	A	C5-N7-C8	8.15	107.98	103.90
1	AA	1275	A	C5-N7-C8	8.15	107.98	103.90
1	AA	1441	A	C5-N7-C8	8.15	107.98	103.90
26	BA	727	A	C5-N7-C8	8.15	107.98	103.90
26	BA	1275	A	C5-N7-C8	8.15	107.98	103.90
26	BA	1932	A	C5-N7-C8	8.15	107.98	103.90
26	BA	1434	A	C5-N7-C8	8.15	107.98	103.90
27	BB	78	A	C5-N7-C8	8.15	107.98	103.90
1	AA	889	A	C5-N7-C8	8.15	107.97	103.90
26	BA	146	A	C5-N7-C8	8.15	107.97	103.90
26	BA	627	A	C5-N7-C8	8.15	107.98	103.90
26	BA	730	A	C5-N7-C8	8.15	107.97	103.90
26	BA	1073	A	C5-N7-C8	8.15	107.97	103.90
26	BA	1504	A	C5-N7-C8	8.15	107.97	103.90
26	BA	1802	A	C5-N7-C8	8.15	107.97	103.90
1	AA	143	A	C5-N7-C8	8.15	107.97	103.90
1	AA	236	A	C5-N7-C8	8.15	107.97	103.90
1	AA	487	A	C5-N7-C8	8.15	107.97	103.90
1	AA	539	A	C5-N7-C8	8.15	107.97	103.90
1	AA	969	A	C5-N7-C8	8.15	107.97	103.90
1	AA	1188	A	C5-N7-C8	8.15	107.97	103.90
26	BA	1689	A	C5-N7-C8	8.15	107.97	103.90
26	BA	2639	A	C5-N7-C8	8.15	107.97	103.90
26	BA	2887	A	C5-N7-C8	8.15	107.97	103.90
1	AA	790	A	C5-N7-C8	8.15	107.97	103.90
26	BA	734	A	C5-N7-C8	8.15	107.97	103.90
26	BA	983	A	C5-N7-C8	8.15	107.97	103.90
26	BA	2670	A	C5-N7-C8	8.15	107.97	103.90
1	AA	174	A	C5-N7-C8	8.14	107.97	103.90
1	AA	547	A	C5-N7-C8	8.14	107.97	103.90
1	AA	784	A	C5-N7-C8	8.14	107.97	103.90
1	AA	914	A	C5-N7-C8	8.14	107.97	103.90
1	AA	1274	A	C5-N7-C8	8.14	107.97	103.90
22	AV	15	A	C5-N7-C8	8.14	107.97	103.90
22	AV	19	A	C5-N7-C8	8.14	107.97	103.90
26	BA	199	A	C5-N7-C8	8.14	107.97	103.90
26	BA	1302	A	C5-N7-C8	8.14	107.97	103.90
26	BA	1403	A	C5-N7-C8	8.14	107.97	103.90
26	BA	1470	A	C5-N7-C8	8.14	107.97	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	250	A	C5-N7-C8	8.14	107.97	103.90
1	AA	313	A	C5-N7-C8	8.14	107.97	103.90
1	AA	777	A	C5-N7-C8	8.14	107.97	103.90
1	AA	1254	A	C5-N7-C8	8.14	107.97	103.90
1	AA	1363	A	C5-N7-C8	8.14	107.97	103.90
26	BA	1009	A	C5-N7-C8	8.14	107.97	103.90
26	BA	1241	A	C5-N7-C8	8.14	107.97	103.90
26	BA	2119	A	C5-N7-C8	8.14	107.97	103.90
26	BA	2614	A	C5-N7-C8	8.14	107.97	103.90
26	BA	1342	A	C5-N7-C8	8.14	107.97	103.90
26	BA	2706	A	C5-N7-C8	8.14	107.97	103.90
1	AA	1480	A	C5-N7-C8	8.14	107.97	103.90
26	BA	203	A	C5-N7-C8	8.14	107.97	103.90
1	AA	101	A	C5-N7-C8	8.14	107.97	103.90
1	AA	190	A	C5-N7-C8	8.14	107.97	103.90
26	BA	173	A	C5-N7-C8	8.14	107.97	103.90
26	BA	668	A	C5-N7-C8	8.14	107.97	103.90
26	BA	749	A	C5-N7-C8	8.14	107.97	103.90
26	BA	866	A	C5-N7-C8	8.14	107.97	103.90
26	BA	1981	A	C5-N7-C8	8.14	107.97	103.90
26	BA	2448	A	C5-N7-C8	8.14	107.97	103.90
26	BA	2733	A	C5-N7-C8	8.14	107.97	103.90
1	AA	149	A	C5-N7-C8	8.13	107.97	103.90
1	AA	321	A	C5-N7-C8	8.14	107.97	103.90
1	AA	712	A	C5-N7-C8	8.13	107.97	103.90
26	BA	346	A	C5-N7-C8	8.14	107.97	103.90
26	BA	422	A	C5-N7-C8	8.13	107.97	103.90
26	BA	497	A	C5-N7-C8	8.14	107.97	103.90
26	BA	1570	A	C5-N7-C8	8.13	107.97	103.90
26	BA	2052	A	C5-N7-C8	8.13	107.97	103.90
26	BA	2095	A	C5-N7-C8	8.13	107.97	103.90
26	BA	2205	A	C5-N7-C8	8.13	107.97	103.90
26	BA	2366	A	C5-N7-C8	8.13	107.97	103.90
27	BB	101	A	C5-N7-C8	8.13	107.97	103.90
1	AA	768	A	C5-N7-C8	8.13	107.97	103.90
26	BA	14	A	C5-N7-C8	8.13	107.97	103.90
1	AA	906	A	C5-N7-C8	8.13	107.97	103.90
26	BA	1286	A	C5-N7-C8	8.13	107.97	103.90
26	BA	616	A	C5-N7-C8	8.13	107.97	103.90
26	BA	1618	A	C5-N7-C8	8.13	107.97	103.90
26	BA	1784	A	C5-N7-C8	8.13	107.97	103.90
26	BA	1912	A	C5-N7-C8	8.13	107.97	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2088	A	C5-N7-C8	8.13	107.97	103.90
26	BA	2660	A	C5-N7-C8	8.13	107.97	103.90
26	BA	2273	A	C5-N7-C8	8.13	107.97	103.90
27	BB	94	A	C5-N7-C8	8.13	107.97	103.90
1	AA	279	A	C5-N7-C8	8.13	107.96	103.90
1	AA	600	A	C5-N7-C8	8.13	107.97	103.90
26	BA	677	A	C5-N7-C8	8.13	107.97	103.90
26	BA	761	A	C5-N7-C8	8.13	107.97	103.90
1	AA	338	A	C5-N7-C8	8.13	107.96	103.90
1	AA	1016	A	C5-N7-C8	8.13	107.96	103.90
1	AA	1271	A	C5-N7-C8	8.13	107.96	103.90
26	BA	2135	A	C5-N7-C8	8.13	107.97	103.90
1	AA	1306	A	C5-N7-C8	8.13	107.96	103.90
25	AY	41	A	C5-N7-C8	8.13	107.96	103.90
26	BA	52	A	C5-N7-C8	8.13	107.96	103.90
26	BA	279	A	C5-N7-C8	8.13	107.96	103.90
26	BA	1155	A	C5-N7-C8	8.13	107.97	103.90
26	BA	1439	A	C5-N7-C8	8.13	107.96	103.90
26	BA	1469	A	C5-N7-C8	8.13	107.96	103.90
1	AA	119	A	C5-N7-C8	8.12	107.96	103.90
1	AA	415	A	C5-N7-C8	8.12	107.96	103.90
1	AA	704	A	C5-N7-C8	8.13	107.96	103.90
1	AA	845	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1256	A	C5-N7-C8	8.12	107.96	103.90
26	BA	94	A	C5-N7-C8	8.13	107.96	103.90
26	BA	1244	A	C5-N7-C8	8.13	107.96	103.90
23	AW	31	A	C5-N7-C8	8.12	107.96	103.90
26	BA	219	A	C5-N7-C8	8.12	107.96	103.90
26	BA	362	A	C5-N7-C8	8.12	107.96	103.90
26	BA	478	A	C5-N7-C8	8.12	107.96	103.90
26	BA	592	A	C5-N7-C8	8.13	107.96	103.90
26	BA	756	A	C5-N7-C8	8.13	107.96	103.90
26	BA	1549	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1978	A	C5-N7-C8	8.12	107.96	103.90
27	BB	66	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1005	A	C5-N7-C8	8.12	107.96	103.90
23	AW	73	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1365	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1456	A	C5-N7-C8	8.12	107.96	103.90
25	AY	66	A	C5-N7-C8	8.12	107.96	103.90
25	AY	73	A	C5-N7-C8	8.12	107.96	103.90
26	BA	221	A	C5-N7-C8	8.12	107.96	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2412	A	C5-N7-C8	8.12	107.96	103.90
26	BA	2497	A	C5-N7-C8	8.12	107.96	103.90
26	BA	44	A	C5-N7-C8	8.12	107.96	103.90
26	BA	472	A	C5-N7-C8	8.12	107.96	103.90
26	BA	661	A	C5-N7-C8	8.12	107.96	103.90
26	BA	675	A	C5-N7-C8	8.12	107.96	103.90
26	BA	941	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1616	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1635	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1819	A	C5-N7-C8	8.12	107.96	103.90
26	BA	2711	A	C5-N7-C8	8.12	107.96	103.90
1	AA	303	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1022	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1046	A	C5-N7-C8	8.12	107.96	103.90
26	BA	654	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1548	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1434	A	C5-N7-C8	8.12	107.96	103.90
26	BA	104	A	C5-N7-C8	8.12	107.96	103.90
26	BA	504	A	C5-N7-C8	8.12	107.96	103.90
26	BA	925	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1373	A	C5-N7-C8	8.12	107.96	103.90
26	BA	368	A	C5-N7-C8	8.12	107.96	103.90
26	BA	626	A	C5-N7-C8	8.12	107.96	103.90
26	BA	716	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1490	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1036	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1201	A	C5-N7-C8	8.12	107.96	103.90
25	AY	21	A	C5-N7-C8	8.12	107.96	103.90
25	AY	58	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1090	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1095	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1214	A	C5-N7-C8	8.12	107.96	103.90
26	BA	1815	A	C5-N7-C8	8.12	107.96	103.90
27	BB	46	A	C5-N7-C8	8.12	107.96	103.90
26	BA	2030	A	C5-N7-C8	8.11	107.96	103.90
26	BA	2679	A	C5-N7-C8	8.12	107.96	103.90
1	AA	28	A	C5-N7-C8	8.11	107.96	103.90
1	AA	160	A	C5-N7-C8	8.11	107.96	103.90
1	AA	1447	A	C5-N7-C8	8.11	107.96	103.90
1	AA	1519	A	C5-N7-C8	8.11	107.96	103.90
26	BA	909	A	C5-N7-C8	8.11	107.96	103.90
26	BA	1580	A	C5-N7-C8	8.11	107.96	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	69	A	C5-N7-C8	8.11	107.95	103.90
26	BA	1515	A	C5-N7-C8	8.11	107.95	103.90
26	BA	2453	A	C5-N7-C8	8.11	107.96	103.90
27	BB	39	A	C5-N7-C8	8.11	107.96	103.90
26	BA	2564	A	C5-N7-C8	8.11	107.95	103.90
1	AA	374	A	C5-N7-C8	8.11	107.95	103.90
23	AW	9	A	C5-N7-C8	8.11	107.95	103.90
26	BA	262	A	C5-N7-C8	8.11	107.95	103.90
26	BA	1321	A	C5-N7-C8	8.11	107.95	103.90
1	AA	715	A	C5-N7-C8	8.11	107.95	103.90
1	AA	1216	A	C5-N7-C8	8.11	107.95	103.90
1	AA	1437	A	C5-N7-C8	8.11	107.95	103.90
26	BA	575	A	C5-N7-C8	8.11	107.95	103.90
26	BA	2015	A	C5-N7-C8	8.11	107.95	103.90
26	BA	2071	A	C5-N7-C8	8.11	107.95	103.90
26	BA	2810	A	C5-N7-C8	8.11	107.95	103.90
1	AA	596	A	C5-N7-C8	8.11	107.95	103.90
26	BA	1759	A	C5-N7-C8	8.11	107.95	103.90
26	BA	1780	A	C5-N7-C8	8.11	107.95	103.90
26	BA	2005	A	C5-N7-C8	8.11	107.95	103.90
1	AA	935	A	C5-N7-C8	8.11	107.95	103.90
1	AA	1093	A	C5-N7-C8	8.11	107.95	103.90
24	AX	76	A	C5-N7-C8	8.11	107.95	103.90
26	BA	1264	A	C5-N7-C8	8.11	107.95	103.90
26	BA	1713	A	C5-N7-C8	8.11	107.95	103.90
26	BA	2886	A	C5-N7-C8	8.11	107.95	103.90
1	AA	81	A	C5-N7-C8	8.10	107.95	103.90
1	AA	306	A	C5-N7-C8	8.10	107.95	103.90
1	AA	574	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1677	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1082	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1169	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1531	A	C5-N7-C8	8.10	107.95	103.90
26	BA	244	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1735	A	C5-N7-C8	8.10	107.95	103.90
26	BA	574	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1020	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1067	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1246	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1347	A	C5-N7-C8	8.10	107.95	103.90
27	BB	115	A	C5-N7-C8	8.10	107.95	103.90
1	AA	298	A	C5-N7-C8	8.10	107.95	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1430	A	C5-N7-C8	8.10	107.95	103.90
1	AA	675	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1110	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1261	A	C5-N7-C8	8.10	107.95	103.90
26	BA	272	A	C5-N7-C8	8.10	107.95	103.90
26	BA	309	A	C5-N7-C8	8.10	107.95	103.90
26	BA	412	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1265	A	C5-N7-C8	8.10	107.95	103.90
26	BA	447	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1900	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1927	A	C5-N7-C8	8.10	107.95	103.90
26	BA	2792	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1101	A	C5-N7-C8	8.10	107.95	103.90
26	BA	218	A	C5-N7-C8	8.10	107.95	103.90
26	BA	590	A	C5-N7-C8	8.10	107.95	103.90
26	BA	820	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1028	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1453	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1665	A	C5-N7-C8	8.10	107.95	103.90
26	BA	1829	A	C5-N7-C8	8.10	107.95	103.90
26	BA	2054	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1227	A	C5-N7-C8	8.09	107.95	103.90
26	BA	1395	A	C5-N7-C8	8.09	107.95	103.90
26	BA	1596	A	C5-N7-C8	8.09	107.95	103.90
26	BA	2587	A	C5-N7-C8	8.09	107.95	103.90
26	BA	2837	A	C5-N7-C8	8.09	107.95	103.90
26	BA	928	A	C5-N7-C8	8.09	107.95	103.90
26	BA	2654	A	C5-N7-C8	8.09	107.95	103.90
1	AA	327	A	C5-N7-C8	8.09	107.95	103.90
1	AA	393	A	C5-N7-C8	8.09	107.94	103.90
1	AA	1446	A	C5-N7-C8	8.09	107.94	103.90
26	BA	83	A	C5-N7-C8	8.09	107.94	103.90
26	BA	213	A	C5-N7-C8	8.09	107.94	103.90
26	BA	1129	A	C5-N7-C8	8.09	107.94	103.90
26	BA	1327	A	C5-N7-C8	8.09	107.95	103.90
26	BA	2478	A	C5-N7-C8	8.09	107.95	103.90
1	AA	66	A	C5-N7-C8	8.09	107.94	103.90
1	AA	344	A	C5-N7-C8	8.09	107.94	103.90
1	AA	353	A	C5-N7-C8	8.09	107.94	103.90
1	AA	560	A	C5-N7-C8	8.09	107.94	103.90
26	BA	294	A	C5-N7-C8	8.09	107.94	103.90
26	BA	637	A	C5-N7-C8	8.09	107.94	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1084	A	C5-N7-C8	8.09	107.94	103.90
26	BA	1679	A	C5-N7-C8	8.09	107.94	103.90
1	AA	172	A	C5-N7-C8	8.09	107.94	103.90
26	BA	330	A	C5-N7-C8	8.09	107.94	103.90
26	BA	1077	A	C5-N7-C8	8.09	107.94	103.90
26	BA	1608	A	C5-N7-C8	8.09	107.94	103.90
26	BA	1392	A	C5-N7-C8	8.09	107.94	103.90
27	BB	104	A	C5-N7-C8	8.09	107.94	103.90
26	BA	1098	A	C5-N7-C8	8.08	107.94	103.90
1	AA	77	A	C5-N7-C8	8.08	107.94	103.90
1	AA	533	A	C5-N7-C8	8.08	107.94	103.90
1	AA	780	A	C5-N7-C8	8.08	107.94	103.90
1	AA	1285	A	C5-N7-C8	8.08	107.94	103.90
1	AA	1375	A	C5-N7-C8	8.08	107.94	103.90
1	AA	1508	A	C5-N7-C8	8.08	107.94	103.90
22	AV	20	A	C5-N7-C8	8.08	107.94	103.90
26	BA	156	A	C5-N7-C8	8.08	107.94	103.90
26	BA	429	A	C5-N7-C8	8.08	107.94	103.90
26	BA	522	A	C5-N7-C8	8.08	107.94	103.90
26	BA	751	A	C5-N7-C8	8.08	107.94	103.90
26	BA	1253	A	C5-N7-C8	8.08	107.94	103.90
26	BA	1579	A	C5-N7-C8	8.08	107.94	103.90
26	BA	1858	A	C5-N7-C8	8.08	107.94	103.90
26	BA	2199	A	C5-N7-C8	8.08	107.94	103.90
26	BA	2425	A	C5-N7-C8	8.08	107.94	103.90
1	AA	642	A	C5-N7-C8	8.08	107.94	103.90
1	AA	1171	A	C5-N7-C8	8.08	107.94	103.90
26	BA	21	A	C5-N7-C8	8.08	107.94	103.90
26	BA	844	A	C5-N7-C8	8.08	107.94	103.90
26	BA	1495	A	C5-N7-C8	8.08	107.94	103.90
26	BA	2407	A	C5-N7-C8	8.08	107.94	103.90
26	BA	1413	A	C5-N7-C8	8.08	107.94	103.90
26	BA	2820	A	C5-N7-C8	8.08	107.94	103.90
1	AA	382	A	C5-N7-C8	8.08	107.94	103.90
1	AA	468	A	C5-N7-C8	8.08	107.94	103.90
1	AA	482	A	C5-N7-C8	8.08	107.94	103.90
1	AA	787	A	C5-N7-C8	8.08	107.94	103.90
1	AA	1004	A	C5-N7-C8	8.08	107.94	103.90
26	BA	721	A	C5-N7-C8	8.08	107.94	103.90
26	BA	1000	A	C5-N7-C8	8.08	107.94	103.90
1	AA	1163	A	C5-N7-C8	8.08	107.94	103.90
26	BA	1583	A	C5-N7-C8	8.08	107.94	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1787	A	C5-N7-C8	8.08	107.94	103.90
26	BA	2541	A	C5-N7-C8	8.08	107.94	103.90
26	BA	2635	A	C5-N7-C8	8.08	107.94	103.90
26	BA	2883	A	C5-N7-C8	8.08	107.94	103.90
1	AA	315	A	C5-N7-C8	8.07	107.94	103.90
1	AA	816	A	C5-N7-C8	8.07	107.94	103.90
1	AA	1092	A	C5-N7-C8	8.07	107.94	103.90
26	BA	2227	A	C5-N7-C8	8.07	107.94	103.90
1	AA	609	A	C5-N7-C8	8.07	107.94	103.90
23	AW	66	A	C5-N7-C8	8.07	107.94	103.90
26	BA	735	A	C5-N7-C8	8.07	107.94	103.90
26	BA	1156	A	C5-N7-C8	8.07	107.94	103.90
26	BA	2059	A	C5-N7-C8	8.07	107.94	103.90
1	AA	975	A	C5-N7-C8	8.07	107.94	103.90
26	BA	753	A	C5-N7-C8	8.07	107.94	103.90
26	BA	789	A	C5-N7-C8	8.07	107.94	103.90
26	BA	2749	A	C5-N7-C8	8.07	107.94	103.90
1	AA	523	A	C5-N7-C8	8.07	107.94	103.90
1	AA	909	A	C5-N7-C8	8.07	107.94	103.90
1	AA	1289	A	C5-N7-C8	8.07	107.94	103.90
26	BA	896	A	C5-N7-C8	8.07	107.94	103.90
26	BA	1528	A	C5-N7-C8	8.07	107.94	103.90
26	BA	1586	A	C5-N7-C8	8.07	107.94	103.90
1	AA	16	A	C5-N7-C8	8.07	107.93	103.90
1	AA	33	A	C5-N7-C8	8.07	107.93	103.90
1	AA	478	A	C5-N7-C8	8.07	107.93	103.90
1	AA	729	A	C5-N7-C8	8.07	107.93	103.90
1	AA	746	A	C5-N7-C8	8.07	107.93	103.90
1	AA	1044	A	C5-N7-C8	8.07	107.93	103.90
1	AA	1130	A	C5-N7-C8	8.07	107.93	103.90
26	BA	324	A	C5-N7-C8	8.07	107.93	103.90
26	BA	980	A	C5-N7-C8	8.07	107.93	103.90
26	BA	988	A	C5-N7-C8	8.07	107.93	103.90
26	BA	1226	A	C5-N7-C8	8.07	107.93	103.90
26	BA	1505	A	C5-N7-C8	8.07	107.93	103.90
26	BA	2278	A	C5-N7-C8	8.07	107.93	103.90
26	BA	1285	A	C5-N7-C8	8.07	107.93	103.90
26	BA	2434	A	C5-N7-C8	8.07	107.93	103.90
1	AA	702	A	C5-N7-C8	8.06	107.93	103.90
1	AA	1067	A	C5-N7-C8	8.06	107.93	103.90
26	BA	311	A	C5-N7-C8	8.06	107.93	103.90
26	BA	892	A	C5-N7-C8	8.06	107.93	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	943	A	C5-N7-C8	8.06	107.93	103.90
26	BA	1328	A	C5-N7-C8	8.06	107.93	103.90
26	BA	1690	A	C5-N7-C8	8.06	107.93	103.90
26	BA	1890	A	C5-N7-C8	8.06	107.93	103.90
1	AA	579	A	C5-N7-C8	8.06	107.93	103.90
1	AA	1534	A	C5-N7-C8	8.06	107.93	103.90
26	BA	670	A	C5-N7-C8	8.06	107.93	103.90
26	BA	1803	A	C5-N7-C8	8.06	107.93	103.90
24	AX	3	A	C5-N7-C8	8.06	107.93	103.90
26	BA	443	A	C5-N7-C8	8.06	107.93	103.90
1	AA	336	A	C5-N7-C8	8.06	107.93	103.90
1	AA	595	A	C5-N7-C8	8.06	107.93	103.90
1	AA	607	A	C5-N7-C8	8.06	107.93	103.90
1	AA	1332	A	C5-N7-C8	8.06	107.93	103.90
26	BA	947	A	C5-N7-C8	8.06	107.93	103.90
26	BA	2225	A	C5-N7-C8	8.06	107.93	103.90
24	AX	23	A	C5-N7-C8	8.06	107.93	103.90
26	BA	63	A	C5-N7-C8	8.06	107.93	103.90
26	BA	1027	A	C5-N7-C8	8.06	107.93	103.90
26	BA	1783	A	C5-N7-C8	8.06	107.93	103.90
26	BA	2547	A	C5-N7-C8	8.06	107.93	103.90
26	BA	1262	A	C5-N7-C8	8.06	107.93	103.90
1	AA	496	A	C5-N7-C8	8.05	107.93	103.90
26	BA	1276	A	C5-N7-C8	8.05	107.93	103.90
26	BA	2826	A	C5-N7-C8	8.05	107.93	103.90
26	BA	1383	A	C5-N7-C8	8.05	107.93	103.90
26	BA	1744	A	C5-N7-C8	8.05	107.93	103.90
26	BA	1889	A	C5-N7-C8	8.05	107.93	103.90
26	BA	2781	A	C5-N7-C8	8.05	107.93	103.90
26	BA	2835	A	C5-N7-C8	8.05	107.93	103.90
1	AA	819	A	C5-N7-C8	8.05	107.93	103.90
26	BA	118	A	C5-N7-C8	8.05	107.92	103.90
26	BA	1204	A	C5-N7-C8	8.05	107.93	103.90
26	BA	972	A	C5-N7-C8	8.05	107.92	103.90
26	BA	1610	A	C5-N7-C8	8.05	107.93	103.90
26	BA	2333	A	C5-N7-C8	8.05	107.92	103.90
26	BA	2369	A	C5-N7-C8	8.05	107.92	103.90
1	AA	510	A	C5-N7-C8	8.05	107.92	103.90
22	AV	21	A	C5-N7-C8	8.05	107.92	103.90
1	AA	964	A	C5-N7-C8	8.05	107.92	103.90
1	AA	1513	A	C5-N7-C8	8.05	107.92	103.90
26	BA	1477	A	C5-N7-C8	8.05	107.92	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1668	A	C5-N7-C8	8.05	107.92	103.90
26	BA	764	A	C5-N7-C8	8.05	107.92	103.90
26	BA	1151	A	C5-N7-C8	8.05	107.92	103.90
26	BA	1269	A	C5-N7-C8	8.05	107.92	103.90
26	BA	2809	A	C5-N7-C8	8.05	107.92	103.90
1	AA	262	A	C5-N7-C8	8.05	107.92	103.90
1	AA	1269	A	C5-N7-C8	8.05	107.92	103.90
26	BA	975	A	C5-N7-C8	8.05	107.92	103.90
26	BA	1672	A	C5-N7-C8	8.05	107.92	103.90
26	BA	1701	A	C5-N7-C8	8.05	107.92	103.90
1	AA	1319	A	C5-N7-C8	8.04	107.92	103.90
1	AA	1465	A	C5-N7-C8	8.04	107.92	103.90
26	BA	984	A	C5-N7-C8	8.04	107.92	103.90
26	BA	1885	A	C5-N7-C8	8.04	107.92	103.90
26	BA	282	A	C5-N7-C8	8.04	107.92	103.90
26	BA	1088	A	C5-N7-C8	8.04	107.92	103.90
26	BA	1928	A	C5-N7-C8	8.04	107.92	103.90
26	BA	1977	A	C5-N7-C8	8.04	107.92	103.90
26	BA	404	A	C5-N7-C8	8.04	107.92	103.90
26	BA	2042	A	C5-N7-C8	8.04	107.92	103.90
26	BA	2212	A	C5-N7-C8	8.04	107.92	103.90
26	BA	2376	A	C5-N7-C8	8.04	107.92	103.90
26	BA	2336	A	C5-N7-C8	8.04	107.92	103.90
26	BA	2725	A	C5-N7-C8	8.04	107.92	103.90
26	BA	2856	A	C5-N7-C8	8.04	107.92	103.90
1	AA	1180	A	C5-N7-C8	8.04	107.92	103.90
26	BA	722	A	C5-N7-C8	8.04	107.92	103.90
26	BA	2430	A	C5-N7-C8	8.04	107.92	103.90
1	AA	1035	A	C5-N7-C8	8.04	107.92	103.90
24	AX	24	A	C5-N7-C8	8.04	107.92	103.90
26	BA	227	A	C5-N7-C8	8.04	107.92	103.90
26	BA	572	A	C5-N7-C8	8.04	107.92	103.90
26	BA	643	A	C5-N7-C8	8.04	107.92	103.90
26	BA	1393	A	C5-N7-C8	8.04	107.92	103.90
26	BA	1591	A	C5-N7-C8	8.04	107.92	103.90
26	BA	990	A	C5-N7-C8	8.04	107.92	103.90
26	BA	2158	A	C5-N7-C8	8.04	107.92	103.90
26	BA	2741	A	C5-N7-C8	8.04	107.92	103.90
26	BA	423	A	C5-N7-C8	8.03	107.92	103.90
26	BA	515	A	C5-N7-C8	8.03	107.92	103.90
26	BA	1525	A	C5-N7-C8	8.04	107.92	103.90
26	BA	2163	A	C5-N7-C8	8.04	107.92	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2468	A	C5-N7-C8	8.03	107.92	103.90
1	AA	2	A	C5-N7-C8	8.03	107.92	103.90
1	AA	559	A	C5-N7-C8	8.03	107.92	103.90
1	AA	1157	A	C5-N7-C8	8.03	107.92	103.90
26	BA	1936	A	C5-N7-C8	8.03	107.92	103.90
1	AA	26	A	C5-N7-C8	8.03	107.92	103.90
1	AA	195	A	C5-N7-C8	8.03	107.92	103.90
1	AA	1507	A	C5-N7-C8	8.03	107.92	103.90
26	BA	1133	A	C5-N7-C8	8.03	107.92	103.90
26	BA	1274	A	C5-N7-C8	8.03	107.92	103.90
26	BA	2184	A	C5-N7-C8	8.03	107.92	103.90
26	BA	2191	A	C5-N7-C8	8.03	107.92	103.90
1	AA	495	A	C5-N7-C8	8.03	107.92	103.90
1	AA	32	A	C5-N7-C8	8.03	107.91	103.90
1	AA	205	A	C5-N7-C8	8.03	107.91	103.90
1	AA	996	A	C5-N7-C8	8.03	107.91	103.90
26	BA	342	A	C5-N7-C8	8.03	107.91	103.90
26	BA	1762	A	C5-N7-C8	8.03	107.92	103.90
1	AA	161	A	C5-N7-C8	8.03	107.91	103.90
1	AA	171	A	C5-N7-C8	8.03	107.91	103.90
1	AA	1333	A	C5-N7-C8	8.03	107.91	103.90
26	BA	563	A	C5-N7-C8	8.03	107.91	103.90
26	BA	13	A	C5-N7-C8	8.03	107.91	103.90
26	BA	715	A	C5-N7-C8	8.03	107.91	103.90
26	BA	2037	A	C5-N7-C8	8.03	107.91	103.90
26	BA	2062	A	C5-N7-C8	8.03	107.91	103.90
27	BB	45	A	C5-N7-C8	8.03	107.91	103.90
1	AA	192	A	C5-N7-C8	8.02	107.91	103.90
1	AA	1081	A	C5-N7-C8	8.02	107.91	103.90
26	BA	1021	A	C5-N7-C8	8.02	107.91	103.90
1	AA	71	A	C5-N7-C8	8.02	107.91	103.90
1	AA	728	A	C5-N7-C8	8.02	107.91	103.90
1	AA	356	A	C5-N7-C8	8.02	107.91	103.90
1	AA	958	A	C5-N7-C8	8.02	107.91	103.90
1	AA	1396	A	C5-N7-C8	8.02	107.91	103.90
26	BA	322	A	C5-N7-C8	8.02	107.91	103.90
26	BA	920	A	C5-N7-C8	8.02	107.91	103.90
26	BA	2340	A	C5-N7-C8	8.02	107.91	103.90
26	BA	2800	A	C5-N7-C8	8.02	107.91	103.90
1	AA	238	A	C5-N7-C8	8.02	107.91	103.90
26	BA	2439	A	C5-N7-C8	8.02	107.91	103.90
26	BA	2813	A	C5-N7-C8	8.02	107.91	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	509	A	C5-N7-C8	8.01	107.91	103.90
1	AA	977	A	C5-N7-C8	8.01	107.91	103.90
1	AA	1346	A	C5-N7-C8	8.01	107.91	103.90
1	AA	1431	A	C5-N7-C8	8.01	107.91	103.90
25	AY	9	A	C5-N7-C8	8.01	107.91	103.90
26	BA	2274	A	C5-N7-C8	8.01	107.91	103.90
26	BA	1086	A	C5-N7-C8	8.01	107.91	103.90
26	BA	2764	A	C5-N7-C8	8.01	107.91	103.90
1	AA	1191	A	C5-N7-C8	8.01	107.91	103.90
26	BA	2051	A	C5-N7-C8	8.01	107.91	103.90
26	BA	2094	A	C5-N7-C8	8.01	107.91	103.90
26	BA	300	A	C5-N7-C8	8.01	107.91	103.90
26	BA	2297	A	C5-N7-C8	8.01	107.91	103.90
27	BB	50	A	C5-N7-C8	8.01	107.91	103.90
27	BB	99	A	C5-N7-C8	8.01	107.91	103.90
1	AA	3	A	C5-N7-C8	8.01	107.90	103.90
1	AA	520	A	C5-N7-C8	8.01	107.90	103.90
26	BA	1001	A	C5-N7-C8	8.01	107.90	103.90
26	BA	1384	A	C5-N7-C8	8.01	107.90	103.90
26	BA	2799	A	C5-N7-C8	8.01	107.90	103.90
1	AA	1219	A	C5-N7-C8	8.01	107.90	103.90
26	BA	586	A	C5-N7-C8	8.01	107.90	103.90
26	BA	782	A	C5-N7-C8	8.01	107.90	103.90
26	BA	1322	A	C5-N7-C8	8.01	107.90	103.90
26	BA	2169	A	C5-N7-C8	8.01	107.90	103.90
26	BA	532	A	C5-N7-C8	8.00	107.90	103.90
26	BA	631	A	C5-N7-C8	8.00	107.90	103.90
26	BA	911	A	C5-N7-C8	8.00	107.90	103.90
26	BA	973	A	C5-N7-C8	8.00	107.90	103.90
26	BA	2386	A	C5-N7-C8	8.00	107.90	103.90
26	BA	2879	A	C5-N7-C8	8.00	107.90	103.90
1	AA	1350	A	C5-N7-C8	8.00	107.90	103.90
26	BA	793	A	C5-N7-C8	8.00	107.90	103.90
26	BA	2432	A	C5-N7-C8	8.00	107.90	103.90
1	AA	270	A	C5-N7-C8	8.00	107.90	103.90
1	AA	919	A	C5-N7-C8	8.00	107.90	103.90
27	BB	57	A	C5-N7-C8	8.00	107.90	103.90
1	AA	459	A	C5-N7-C8	8.00	107.90	103.90
26	BA	207	A	C5-N7-C8	8.00	107.90	103.90
26	BA	1711	A	C5-N7-C8	8.00	107.90	103.90
26	BA	1810	A	C5-N7-C8	8.00	107.90	103.90
26	BA	2317	A	C5-N7-C8	8.00	107.90	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1170	A	C5-N7-C8	7.99	107.90	103.90
26	BA	1866	A	C5-N7-C8	7.99	107.90	103.90
1	AA	532	A	C5-N7-C8	7.99	107.90	103.90
26	BA	514	A	C5-N7-C8	7.99	107.90	103.90
26	BA	1039	A	C5-N7-C8	7.99	107.90	103.90
1	AA	498	A	C5-N7-C8	7.99	107.89	103.90
1	AA	1014	A	C5-N7-C8	7.99	107.89	103.90
23	AW	76	A	C5-N7-C8	7.99	107.89	103.90
26	BA	689	A	C5-N7-C8	7.99	107.90	103.90
26	BA	2171	A	C5-N7-C8	7.99	107.89	103.90
26	BA	2378	A	C5-N7-C8	7.99	107.89	103.90
26	BA	821	A	C5-N7-C8	7.99	107.89	103.90
26	BA	1433	A	C5-N7-C8	7.99	107.89	103.90
1	AA	1167	A	C5-N7-C8	7.99	107.89	103.90
26	BA	1387	A	C5-N7-C8	7.99	107.89	103.90
1	AA	864	A	C5-N7-C8	7.99	107.89	103.90
26	BA	56	A	C5-N7-C8	7.99	107.89	103.90
26	BA	845	A	C5-N7-C8	7.99	107.89	103.90
26	BA	1419	A	C5-N7-C8	7.99	107.89	103.90
26	BA	1632	A	C5-N7-C8	7.99	107.89	103.90
1	AA	364	A	C5-N7-C8	7.98	107.89	103.90
26	BA	1284	A	C5-N7-C8	7.98	107.89	103.90
26	BA	2114	A	C5-N7-C8	7.98	107.89	103.90
26	BA	2266	A	C5-N7-C8	7.98	107.89	103.90
1	AA	282	A	C5-N7-C8	7.98	107.89	103.90
1	AA	983	A	C5-N7-C8	7.98	107.89	103.90
1	AA	1145	A	C5-N7-C8	7.98	107.89	103.90
26	BA	10	A	C5-N7-C8	7.98	107.89	103.90
26	BA	1626	A	C5-N7-C8	7.98	107.89	103.90
26	BA	2565	A	C5-N7-C8	7.98	107.89	103.90
1	AA	493	A	C5-N7-C8	7.97	107.89	103.90
26	BA	226	A	C5-N7-C8	7.97	107.89	103.90
1	AA	665	A	C5-N7-C8	7.97	107.89	103.90
26	BA	2531	A	C5-N7-C8	7.97	107.89	103.90
26	BA	2868	A	C5-N7-C8	7.97	107.89	103.90
1	AA	1288	A	C5-N7-C8	7.97	107.88	103.90
26	BA	2267	A	C5-N7-C8	7.97	107.88	103.90
22	AV	17	A	C5-N7-C8	7.97	107.88	103.90
26	BA	676	A	C5-N7-C8	7.97	107.88	103.90
1	AA	451	A	C5-N7-C8	7.96	107.88	103.90
26	BA	1496	A	C5-N7-C8	7.96	107.88	103.90
1	AA	814	A	C5-N7-C8	7.96	107.88	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	127	A	C5-N7-C8	7.96	107.88	103.90
26	BA	167	A	C5-N7-C8	7.96	107.88	103.90
26	BA	2097	A	C5-N7-C8	7.96	107.88	103.90
26	BA	2675	A	C5-N7-C8	7.96	107.88	103.90
26	BA	960	A	C5-N7-C8	7.96	107.88	103.90
26	BA	582	A	C5-N7-C8	7.96	107.88	103.90
26	BA	1598	A	C5-N7-C8	7.96	107.88	103.90
26	BA	685	A	C5-N7-C8	7.96	107.88	103.90
26	BA	750	A	C5-N7-C8	7.96	107.88	103.90
27	BB	73	A	C5-N7-C8	7.95	107.88	103.90
26	BA	743	A	C5-N7-C8	7.95	107.88	103.90
26	BA	1378	A	C5-N7-C8	7.95	107.88	103.90
26	BA	1854	A	C5-N7-C8	7.95	107.88	103.90
26	BA	2860	A	C5-N7-C8	7.95	107.88	103.90
26	BA	2872	A	C5-N7-C8	7.95	107.88	103.90
1	AA	1238	A	C5-N7-C8	7.95	107.87	103.90
1	AA	608	A	C5-N7-C8	7.94	107.87	103.90
26	BA	1789	A	C5-N7-C8	7.94	107.87	103.90
26	BA	2392	A	C5-N7-C8	7.94	107.87	103.90
26	BA	613	A	C5-N7-C8	7.94	107.87	103.90
26	BA	503	A	C5-N7-C8	7.94	107.87	103.90
1	AA	412	A	C5-N7-C8	7.94	107.87	103.90
1	AA	563	A	C5-N7-C8	7.93	107.87	103.90
1	AA	923	A	C5-N7-C8	7.93	107.87	103.90
1	AA	1021	A	C5-N7-C8	7.93	107.87	103.90
1	AA	1324	A	C5-N7-C8	7.93	107.87	103.90
26	BA	863	A	C5-N7-C8	7.93	107.87	103.90
26	BA	2459	A	C5-N7-C8	7.93	107.87	103.90
1	AA	766	A	C5-N7-C8	7.93	107.87	103.90
26	BA	233	A	C5-N7-C8	7.93	107.87	103.90
26	BA	529	A	C5-N7-C8	7.93	107.87	103.90
1	AA	1080	A	C5-N7-C8	7.93	107.87	103.90
1	AA	1357	A	C5-N7-C8	7.93	107.87	103.90
26	BA	2058	A	C5-N7-C8	7.93	107.86	103.90
26	BA	1096	A	C5-N7-C8	7.93	107.86	103.90
26	BA	1603	A	C5-N7-C8	7.93	107.86	103.90
1	AA	1252	A	C5-N7-C8	7.92	107.86	103.90
26	BA	91	A	C5-N7-C8	7.92	107.86	103.90
26	BA	384	A	C5-N7-C8	7.92	107.86	103.90
26	BA	2823	A	C5-N7-C8	7.92	107.86	103.90
1	AA	116	A	C5-N7-C8	7.92	107.86	103.90
1	AA	1362	A	C5-N7-C8	7.92	107.86	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	119	A	C5-N7-C8	7.92	107.86	103.90
26	BA	1522	A	C5-N7-C8	7.92	107.86	103.90
26	BA	196	A	C5-N7-C8	7.92	107.86	103.90
26	BA	632	A	C5-N7-C8	7.92	107.86	103.90
26	BA	415	A	C5-N7-C8	7.91	107.86	103.90
26	BA	2327	A	C5-N7-C8	7.91	107.86	103.90
26	BA	1872	A	C5-N7-C8	7.91	107.86	103.90
26	BA	2020	A	C5-N7-C8	7.91	107.86	103.90
26	BA	2766	A	C5-N7-C8	7.91	107.86	103.90
26	BA	1010	A	C5-N7-C8	7.91	107.85	103.90
26	BA	2287	A	C5-N7-C8	7.91	107.85	103.90
26	BA	2469	A	C5-N7-C8	7.90	107.85	103.90
1	AA	196	A	C5-N7-C8	7.90	107.85	103.90
26	BA	1953	A	C5-N7-C8	7.90	107.85	103.90
26	BA	1545	A	C5-N7-C8	7.90	107.85	103.90
1	AA	901	A	C5-N7-C8	7.90	107.85	103.90
26	BA	1745	A	C5-N7-C8	7.90	107.85	103.90
1	AA	263	A	C5-N7-C8	7.89	107.85	103.90
26	BA	53	A	C5-N7-C8	7.89	107.85	103.90
26	BA	933	A	C5-N7-C8	7.89	107.85	103.90
26	BA	1669	A	C5-N7-C8	7.89	107.85	103.90
1	AA	397	A	C5-N7-C8	7.89	107.84	103.90
26	BA	2757	A	C5-N7-C8	7.89	107.84	103.90
1	AA	389	A	C5-N7-C8	7.89	107.84	103.90
26	BA	1664	A	C5-N7-C8	7.89	107.84	103.90
26	BA	430	A	C5-N7-C8	7.88	107.84	103.90
26	BA	2080	A	C5-N7-C8	7.88	107.84	103.90
1	AA	622	A	C5-N7-C8	7.88	107.84	103.90
1	AA	865	A	C5-N7-C8	7.88	107.84	103.90
1	AA	959	A	C5-N7-C8	7.88	107.84	103.90
26	BA	2451	A	C5-N7-C8	7.88	107.84	103.90
26	BA	1614	A	C5-N7-C8	7.87	107.84	103.90
26	BA	1676	A	C5-N7-C8	7.87	107.83	103.90
1	AA	1152	A	C5-N7-C8	7.87	107.83	103.90
26	BA	833	A	C5-N7-C8	7.87	107.83	103.90
1	AA	182	A	C5-N7-C8	7.86	107.83	103.90
26	BA	251	A	C5-N7-C8	7.86	107.83	103.90
26	BA	1791	A	C5-N7-C8	7.85	107.83	103.90
26	BA	161	A	C5-N7-C8	7.85	107.83	103.90
26	BA	278	A	C5-N7-C8	7.85	107.83	103.90
26	BA	142	A	C5-N7-C8	7.85	107.82	103.90
26	BA	752	A	C5-N7-C8	7.84	107.82	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1359	A	C5-N7-C8	7.84	107.82	103.90
26	BA	1260	A	C5-N7-C8	7.84	107.82	103.90
26	BA	981	A	C5-N7-C8	7.83	107.82	103.90
26	BA	1901	A	C5-N7-C8	7.83	107.82	103.90
26	BA	2450	A	C5-N7-C8	7.83	107.81	103.90
26	BA	2328	A	C5-N7-C8	7.81	107.81	103.90
26	BA	546	U	C2-N1-C1'	7.81	127.07	117.70
26	BA	1785	A	C5-N7-C8	7.79	107.79	103.90
1	AA	872	A	C5-N7-C8	7.78	107.79	103.90
26	BA	1301	A	C5-N7-C8	7.78	107.79	103.90
1	AA	452	A	C5-N7-C8	7.78	107.79	103.90
26	BA	633	A	C5-N7-C8	7.78	107.79	103.90
26	BA	2598	A	C5-N7-C8	7.77	107.78	103.90
1	AA	430	A	C5-N7-C8	7.76	107.78	103.90
26	BA	1876	A	C5-N7-C8	7.76	107.78	103.90
26	BA	2662	A	C5-N7-C8	7.76	107.78	103.90
26	BA	783	A	C5-N7-C8	7.76	107.78	103.90
26	BA	73	A	C5-N7-C8	7.75	107.77	103.90
26	BA	1899	A	C5-N7-C8	7.74	107.77	103.90
1	AA	546	A	C5-N7-C8	7.73	107.77	103.90
1	AA	502	A	C5-N7-C8	7.71	107.75	103.90
26	BA	528	A	C5-N7-C8	7.63	107.72	103.90
26	BA	466	A	C5-N7-C8	7.61	107.70	103.90
26	BA	278	A	N3-C4-N9	7.58	133.47	127.40
24	AX	19	U	N3-C4-C5	7.58	119.15	114.60
24	AX	16	U	N3-C4-C5	7.55	119.13	114.60
1	AA	754	C	C2-N1-C1'	7.55	127.11	118.80
23	AW	20	U	N3-C4-C5	7.54	119.12	114.60
24	AX	20	U	N3-C4-C5	7.46	119.08	114.60
26	BA	2114	A	N3-C4-N9	7.45	133.36	127.40
1	AA	1158	C	N3-C2-O2	-7.42	116.71	121.90
26	BA	546	U	N1-C2-O2	7.40	127.98	122.80
23	AW	20	U	N3-C2-O2	-7.32	117.08	122.20
24	AX	20	U	N3-C2-O2	-7.32	117.08	122.20
24	AX	16	U	N3-C2-O2	-7.29	117.10	122.20
24	AX	19	U	N3-C2-O2	-7.27	117.11	122.20
1	AA	983	A	N3-C4-N9	7.26	133.21	127.40
26	BA	1313	U	C2-N1-C1'	7.22	126.36	117.70
1	AA	397	A	N3-C4-N9	7.11	133.09	127.40
26	BA	2430	A	N3-C4-N9	7.10	133.08	127.40
26	BA	1570	A	C4-C5-C6	7.10	120.55	117.00
1	AA	754	C	N1-C2-O2	7.09	123.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	633	A	C4-C5-C6	7.07	120.53	117.00
1	AA	408	A	C5-N7-C8	7.06	107.43	103.90
26	BA	1669	A	N3-C4-N9	7.03	133.02	127.40
26	BA	2430	A	C4-C5-C6	7.00	120.50	117.00
26	BA	2077	A	C4-C5-C6	6.97	120.49	117.00
26	BA	2287	A	N3-C4-N9	6.97	132.97	127.40
26	BA	278	A	C4-C5-C6	6.95	120.48	117.00
26	BA	532	A	N3-C4-N9	6.91	132.93	127.40
26	BA	1301	A	N3-C4-N9	6.87	132.89	127.40
1	AA	901	A	C4-C5-C6	6.85	120.43	117.00
1	AA	1005	A	C4-C5-C6	6.82	120.41	117.00
26	BA	1970	A	C4-C5-C6	6.82	120.41	117.00
26	BA	546	U	N3-C2-O2	-6.81	117.43	122.20
26	BA	2114	A	C4-C5-C6	6.76	120.38	117.00
26	BA	2077	A	N3-C4-N9	6.74	132.79	127.40
1	AA	983	A	C4-C5-C6	6.73	120.37	117.00
26	BA	52	A	C4-C5-C6	6.71	120.35	117.00
1	AA	397	A	C4-C5-C6	6.70	120.35	117.00
26	BA	1669	A	C4-C5-C6	6.69	120.34	117.00
26	BA	2267	A	N3-C4-N9	6.69	132.75	127.40
1	AA	563	A	N3-C4-N9	6.66	132.73	127.40
26	BA	960	A	C4-C5-C6	6.66	120.33	117.00
26	BA	633	A	N3-C4-N9	6.66	132.72	127.40
26	BA	819	A	C4-C5-C6	6.65	120.33	117.00
26	BA	2297	A	N3-C4-N9	6.64	132.71	127.40
26	BA	2765	A	N3-C4-N9	6.63	132.70	127.40
1	AA	872	A	N3-C4-N9	6.62	132.70	127.40
26	BA	2297	A	C4-C5-C6	6.61	120.31	117.00
26	BA	2287	A	C4-C5-C6	6.60	120.30	117.00
26	BA	2662	A	C4-C5-C6	6.60	120.30	117.00
27	BB	59	A	N3-C4-N9	6.54	132.63	127.40
1	AA	1167	A	N3-C4-N9	6.54	132.63	127.40
26	BA	1301	A	C4-C5-C6	6.54	120.27	117.00
27	BB	59	A	C4-C5-C6	6.54	120.27	117.00
1	AA	408	A	C4-C5-C6	6.53	120.27	117.00
26	BA	56	A	N3-C4-N9	6.52	132.62	127.40
26	BA	532	A	C4-C5-C6	6.49	120.25	117.00
26	BA	513	A	C4-C5-C6	6.49	120.25	117.00
26	BA	2766	A	N3-C4-N9	6.49	132.59	127.40
26	BA	2765	A	C4-C5-C6	6.48	120.24	117.00
26	BA	2267	A	C4-C5-C6	6.48	120.24	117.00
1	AA	563	A	C4-C5-C6	6.47	120.24	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1029	A	C4-C5-C6	6.47	120.23	117.00
26	BA	330	A	N3-C4-N9	6.47	132.57	127.40
26	BA	1021	A	N3-C4-N9	6.47	132.57	127.40
1	AA	1102	A	N3-C4-N9	6.46	132.57	127.40
26	BA	1535	A	N3-C4-N9	6.46	132.57	127.40
26	BA	1970	A	N3-C4-N9	6.45	132.56	127.40
1	AA	210	C	N3-C2-O2	-6.44	117.39	121.90
23	AW	23	A	C4-C5-C6	6.43	120.22	117.00
26	BA	1553	A	C4-C5-C6	6.43	120.22	117.00
26	BA	819	A	N3-C4-N9	6.43	132.54	127.40
1	AA	977	A	N3-C4-N9	6.42	132.54	127.40
1	AA	1044	A	C4-C5-C6	6.42	120.21	117.00
1	AA	1102	A	C4-C5-C6	6.42	120.21	117.00
26	BA	471	A	C4-C5-C6	6.42	120.21	117.00
1	AA	408	A	N3-C4-N9	6.42	132.54	127.40
1	AA	1044	A	N3-C4-N9	6.42	132.54	127.40
1	AA	908	A	C4-C5-C6	6.42	120.21	117.00
26	BA	933	A	N3-C4-N9	6.42	132.54	127.40
26	BA	1664	A	N3-C4-N9	6.42	132.53	127.40
1	AA	98	A	C4-C5-C6	6.41	120.21	117.00
1	AA	1468	A	C4-C5-C6	6.41	120.20	117.00
26	BA	251	A	C4-C5-C6	6.41	120.20	117.00
26	BA	1570	A	N3-C4-N9	6.41	132.53	127.40
26	BA	1664	A	C4-C5-C6	6.41	120.20	117.00
26	BA	1866	A	C4-C5-C6	6.41	120.20	117.00
26	BA	1395	A	C4-C5-C6	6.40	120.20	117.00
26	BA	1571	A	C4-C5-C6	6.40	120.20	117.00
1	AA	1005	A	N3-C4-N9	6.39	132.51	127.40
26	BA	845	A	C4-C5-C6	6.39	120.20	117.00
1	AA	162	A	C4-C5-C6	6.39	120.19	117.00
26	BA	1213	A	C4-C5-C6	6.39	120.19	117.00
1	AA	190	A	C4-C5-C6	6.39	120.19	117.00
26	BA	2560	A	N3-C4-N9	6.38	132.50	127.40
1	AA	1374	A	C4-C5-C6	6.38	120.19	117.00
26	BA	1021	A	C4-C5-C6	6.38	120.19	117.00
1	AA	98	A	N3-C4-N9	6.37	132.50	127.40
26	BA	1583	A	N3-C4-N9	6.37	132.50	127.40
26	BA	470	A	C4-C5-C6	6.37	120.18	117.00
1	AA	994	A	C4-C5-C6	6.37	120.18	117.00
26	BA	479	A	C8-N9-C4	6.37	108.35	105.80
26	BA	196	A	N3-C4-N9	6.37	132.49	127.40
26	BA	1810	A	C4-C5-C6	6.36	120.18	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	845	A	N3-C4-N9	6.36	132.49	127.40
1	AA	329	A	C4-C5-C6	6.36	120.18	117.00
26	BA	479	A	C4-C5-C6	6.36	120.18	117.00
1	AA	499	A	C8-N9-C4	6.36	108.34	105.80
1	AA	873	A	C4-C5-C6	6.36	120.18	117.00
26	BA	675	A	C4-C5-C6	6.35	120.18	117.00
23	AW	23	A	N3-C4-N9	6.35	132.48	127.40
1	AA	116	A	N3-C4-N9	6.35	132.48	127.40
26	BA	1469	A	C4-C5-C6	6.34	120.17	117.00
26	BA	513	A	N3-C4-N9	6.34	132.47	127.40
26	BA	933	A	C4-C5-C6	6.34	120.17	117.00
26	BA	196	A	C4-C5-C6	6.33	120.17	117.00
1	AA	1418	A	C4-C5-C6	6.33	120.17	117.00
26	BA	2211	A	N3-C4-N9	6.33	132.46	127.40
26	BA	2062	A	N3-C4-N9	6.33	132.46	127.40
26	BA	384	A	N3-C4-N9	6.32	132.46	127.40
1	AA	1157	A	N3-C4-N9	6.32	132.46	127.40
1	AA	116	A	C4-C5-C6	6.32	120.16	117.00
1	AA	539	A	C4-C5-C6	6.31	120.16	117.00
26	BA	330	A	C4-C5-C6	6.31	120.16	117.00
26	BA	599	A	C4-C5-C6	6.31	120.16	117.00
26	BA	2665	A	C4-C5-C6	6.31	120.16	117.00
27	BB	73	A	N3-C4-N9	6.31	132.45	127.40
26	BA	1378	A	N9-C4-C5	6.31	108.32	105.80
26	BA	255	A	C4-C5-C6	6.30	120.15	117.00
26	BA	820	A	C4-C5-C6	6.30	120.15	117.00
1	AA	977	A	C4-C5-C6	6.30	120.15	117.00
26	BA	2412	A	C4-C5-C6	6.30	120.15	117.00
1	AA	1363	A	N3-C4-N9	6.30	132.44	127.40
26	BA	644	A	N3-C4-N9	6.30	132.44	127.40
26	BA	2766	A	C4-C5-C6	6.29	120.15	117.00
26	BA	2335	A	C4-C5-C6	6.29	120.15	117.00
1	AA	923	A	C4-C5-C6	6.29	120.14	117.00
26	BA	572	A	N3-C4-N9	6.29	132.43	127.40
26	BA	2335	A	N3-C4-N9	6.29	132.43	127.40
1	AA	994	A	N3-C4-N9	6.28	132.43	127.40
26	BA	1535	A	C4-C5-C6	6.28	120.14	117.00
1	AA	1363	A	C4-C5-C6	6.28	120.14	117.00
26	BA	2366	A	C4-C5-C6	6.28	120.14	117.00
1	AA	706	A	C4-C5-C6	6.28	120.14	117.00
26	BA	401	A	C4-C5-C6	6.28	120.14	117.00
1	AA	1167	A	C4-C5-C6	6.28	120.14	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	142	A	C4-C5-C6	6.28	120.14	117.00
26	BA	572	A	C4-C5-C6	6.28	120.14	117.00
26	BA	1260	A	C4-C5-C6	6.27	120.14	117.00
26	BA	2662	A	N3-C4-N9	6.27	132.42	127.40
1	AA	872	A	C4-C5-C6	6.27	120.14	117.00
1	AA	1374	A	N3-C4-N9	6.27	132.42	127.40
26	BA	2748	A	C4-C5-C6	6.27	120.14	117.00
1	AA	1299	A	N3-C4-N9	6.27	132.42	127.40
26	BA	404	A	N3-C4-N9	6.27	132.42	127.40
26	BA	863	A	N3-C4-N9	6.27	132.41	127.40
26	BA	1241	A	C4-C5-C6	6.27	120.13	117.00
26	BA	2273	A	C4-C5-C6	6.26	120.13	117.00
26	BA	2407	A	C4-C5-C6	6.26	120.13	117.00
1	AA	495	A	C8-N9-C4	6.26	108.30	105.80
26	BA	56	A	C4-C5-C6	6.26	120.13	117.00
26	BA	142	A	N3-C4-N9	6.26	132.41	127.40
26	BA	362	A	N3-C4-N9	6.26	132.41	127.40
26	BA	2211	A	C4-C5-C6	6.26	120.13	117.00
26	BA	2352	A	C4-C5-C6	6.26	120.13	117.00
26	BA	863	A	C4-C5-C6	6.25	120.13	117.00
1	AA	1339	A	C4-C5-C6	6.25	120.13	117.00
26	BA	1494	A	C4-C5-C6	6.25	120.13	117.00
26	BA	2014	A	C4-C5-C6	6.25	120.13	117.00
1	AA	300	A	C4-C5-C6	6.25	120.12	117.00
1	AA	356	A	C4-C5-C6	6.25	120.12	117.00
26	BA	2560	A	C4-C5-C6	6.25	120.12	117.00
1	AA	907	A	C4-C5-C6	6.24	120.12	117.00
26	BA	1103	A	C4-C5-C6	6.24	120.12	117.00
1	AA	478	A	N3-C4-N9	6.24	132.39	127.40
26	BA	1829	A	N3-C4-N9	6.24	132.39	127.40
26	BA	1969	A	C4-C5-C6	6.24	120.12	117.00
26	BA	2721	A	C4-C5-C6	6.24	120.12	117.00
26	BA	1490	A	N3-C4-N9	6.23	132.39	127.40
26	BA	1784	A	N3-C4-N9	6.23	132.39	127.40
26	BA	756	A	C4-C5-C6	6.23	120.12	117.00
26	BA	1213	A	N3-C4-N9	6.23	132.38	127.40
1	AA	579	A	C4-C5-C6	6.23	120.11	117.00
26	BA	1276	A	N3-C4-N9	6.23	132.38	127.40
1	AA	1157	A	C4-C5-C6	6.23	120.11	117.00
26	BA	1088	A	N3-C4-N9	6.23	132.38	127.40
26	BA	2082	A	C4-C5-C6	6.23	120.11	117.00
1	AA	608	A	N3-C4-N9	6.23	132.38	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1583	A	C4-C5-C6	6.22	120.11	117.00
1	AA	918	A	C4-C5-C6	6.22	120.11	117.00
26	BA	191	A	C4-C5-C6	6.22	120.11	117.00
26	BA	644	A	C4-C5-C6	6.22	120.11	117.00
26	BA	750	A	N3-C4-N9	6.22	132.38	127.40
1	AA	431	A	N9-C4-C5	6.22	108.29	105.80
1	AA	1507	A	N3-C4-N9	6.22	132.37	127.40
1	AA	546	A	C4-C5-C6	6.21	120.11	117.00
1	AA	1158	C	C6-N1-C1'	-6.21	113.34	120.80
26	BA	2062	A	C4-C5-C6	6.21	120.11	117.00
1	AA	1507	A	C4-C5-C6	6.21	120.11	117.00
26	BA	689	A	C4-C5-C6	6.21	120.11	117.00
26	BA	1553	A	N3-C4-N9	6.21	132.37	127.40
1	AA	478	A	C4-C5-C6	6.21	120.10	117.00
26	BA	470	A	N3-C4-N9	6.21	132.37	127.40
26	BA	1313	U	N1-C2-O2	6.21	127.14	122.80
26	BA	1655	A	C8-N9-C4	6.20	108.28	105.80
1	AA	190	A	N3-C4-N9	6.20	132.36	127.40
26	BA	2080	A	C4-C5-C6	6.20	120.10	117.00
1	AA	546	A	N3-C4-N9	6.20	132.36	127.40
26	BA	492	A	C4-C5-C6	6.20	120.10	117.00
26	BA	917	A	C4-C5-C6	6.20	120.10	117.00
26	BA	1829	A	C4-C5-C6	6.20	120.10	117.00
1	AA	694	A	C4-C5-C6	6.20	120.10	117.00
26	BA	64	A	C4-C5-C6	6.20	120.10	117.00
23	AW	20	U	C5-C4-O4	-6.20	122.18	125.90
26	BA	49	A	C4-C5-C6	6.20	120.10	117.00
26	BA	689	A	N3-C4-N9	6.20	132.36	127.40
26	BA	960	A	N3-C4-N9	6.20	132.36	127.40
1	AA	329	A	N3-C4-N9	6.19	132.35	127.40
26	BA	52	A	N3-C4-N9	6.19	132.35	127.40
26	BA	384	A	C4-C5-C6	6.19	120.09	117.00
26	BA	2328	A	C4-C5-C6	6.19	120.09	117.00
1	AA	743	A	C4-C5-C6	6.19	120.09	117.00
26	BA	2799	A	C4-C5-C6	6.19	120.09	117.00
1	AA	1332	A	C4-C5-C6	6.19	120.09	117.00
1	AA	74	A	N9-C4-C5	6.19	108.27	105.80
24	AX	16	U	C5-C4-O4	-6.18	122.19	125.90
26	BA	190	A	C4-C5-C6	6.18	120.09	117.00
1	AA	539	A	N3-C4-N9	6.18	132.35	127.40
1	AA	860	A	C4-C5-C6	6.18	120.09	117.00
26	BA	1244	A	C4-C5-C6	6.18	120.09	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2051	A	C4-C5-C6	6.18	120.09	117.00
26	BA	2665	A	N3-C4-N9	6.18	132.34	127.40
26	BA	1634	A	C4-C5-C6	6.18	120.09	117.00
26	BA	2547	A	C4-C5-C6	6.18	120.09	117.00
26	BA	2823	A	N3-C4-N9	6.18	132.34	127.40
1	AA	509	A	C4-C5-C6	6.18	120.09	117.00
1	AA	1483	A	C4-C5-C6	6.18	120.09	117.00
26	BA	2407	A	N3-C4-N9	6.18	132.34	127.40
26	BA	2799	A	N3-C4-N9	6.18	132.34	127.40
1	AA	448	A	C4-C5-C6	6.18	120.09	117.00
24	AX	19	U	C5-C4-O4	-6.18	122.19	125.90
26	BA	1866	A	N3-C4-N9	6.18	132.34	127.40
26	BA	2171	A	C4-C5-C6	6.18	120.09	117.00
27	BB	99	A	C4-C5-C6	6.18	120.09	117.00
26	BA	231	A	C4-C5-C6	6.17	120.09	117.00
26	BA	1787	A	C4-C5-C6	6.17	120.09	117.00
26	BA	449	A	C4-C5-C6	6.17	120.09	117.00
26	BA	1260	A	N3-C4-N9	6.17	132.34	127.40
1	AA	270	A	C4-C5-C6	6.17	120.09	117.00
26	BA	2451	A	N9-C4-C5	6.17	108.27	105.80
26	BA	401	A	N3-C4-N9	6.17	132.34	127.40
26	BA	794	A	C4-C5-C6	6.17	120.08	117.00
1	AA	1146	A	C4-C5-C6	6.17	120.08	117.00
26	BA	256	A	C4-C5-C6	6.17	120.08	117.00
26	BA	5	A	C4-C5-C6	6.17	120.08	117.00
1	AA	814	A	N3-C4-N9	6.17	132.33	127.40
1	AA	1280	A	C4-C5-C6	6.17	120.08	117.00
1	AA	487	A	C4-C5-C6	6.16	120.08	117.00
1	AA	1468	A	N3-C4-N9	6.16	132.33	127.40
26	BA	2311	A	C4-C5-C6	6.16	120.08	117.00
27	BB	15	A	N3-C4-N9	6.16	132.33	127.40
26	BA	1899	A	C4-C5-C6	6.16	120.08	117.00
1	AA	640	A	C4-C5-C6	6.16	120.08	117.00
1	AA	1329	A	C8-N9-C4	6.16	108.26	105.80
26	BA	685	A	C4-C5-C6	6.16	120.08	117.00
26	BA	706	A	C4-C5-C6	6.16	120.08	117.00
26	BA	1490	A	C4-C5-C6	6.16	120.08	117.00
26	BA	2727	A	C4-C5-C6	6.16	120.08	117.00
26	BA	404	A	C4-C5-C6	6.16	120.08	117.00
26	BA	582	A	C4-C5-C6	6.16	120.08	117.00
26	BA	599	A	N3-C4-N9	6.16	132.33	127.40
26	BA	1787	A	N3-C4-N9	6.16	132.33	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2776	A	C4-C5-C6	6.16	120.08	117.00
1	AA	487	A	N3-C4-N9	6.15	132.32	127.40
26	BA	176	A	C4-C5-C6	6.15	120.08	117.00
1	AA	1357	A	C4-C5-C6	6.15	120.08	117.00
26	BA	233	A	C4-C5-C6	6.15	120.08	117.00
26	BA	632	A	C4-C5-C6	6.15	120.08	117.00
24	AX	20	U	C5-C4-O4	-6.15	122.21	125.90
26	BA	1395	A	N3-C4-N9	6.15	132.32	127.40
1	AA	907	A	N3-C4-N9	6.15	132.32	127.40
26	BA	675	A	N3-C4-N9	6.15	132.32	127.40
26	BA	685	A	N3-C4-N9	6.15	132.32	127.40
26	BA	753	A	C4-C5-C6	6.15	120.07	117.00
26	BA	2748	A	N3-C4-N9	6.15	132.32	127.40
1	AA	356	A	N3-C4-N9	6.14	132.32	127.40
27	BB	52	A	C4-C5-C6	6.14	120.07	117.00
1	AA	1350	A	N3-C4-N9	6.14	132.31	127.40
26	BA	5	A	N3-C4-N9	6.14	132.31	127.40
26	BA	2171	A	N3-C4-N9	6.14	132.31	127.40
26	BA	2800	A	N3-C4-N9	6.14	132.31	127.40
1	AA	695	A	C4-C5-C6	6.14	120.07	117.00
1	AA	814	A	C4-C5-C6	6.14	120.07	117.00
26	BA	1029	A	N3-C4-N9	6.14	132.31	127.40
26	BA	160	A	C4-C5-C6	6.14	120.07	117.00
26	BA	2675	A	N3-C4-N9	6.14	132.31	127.40
26	BA	447	A	C4-C5-C6	6.14	120.07	117.00
26	BA	1353	A	C4-C5-C6	6.14	120.07	117.00
26	BA	2459	A	N3-C4-N9	6.14	132.31	127.40
1	AA	162	A	N3-C4-N9	6.13	132.31	127.40
1	AA	1362	A	C4-C5-C6	6.13	120.07	117.00
26	BA	74	A	C4-C5-C6	6.13	120.07	117.00
26	BA	2163	A	C4-C5-C6	6.13	120.07	117.00
26	BA	2268	A	C4-C5-C6	6.13	120.07	117.00
26	BA	2461	A	N3-C4-N9	6.13	132.31	127.40
26	BA	2547	A	N3-C4-N9	6.13	132.31	127.40
26	BA	255	A	N3-C4-N9	6.13	132.31	127.40
1	AA	270	A	N3-C4-N9	6.13	132.31	127.40
26	BA	1635	A	N3-C4-N9	6.13	132.31	127.40
1	AA	706	A	N3-C4-N9	6.13	132.30	127.40
1	AA	712	A	C4-C5-C6	6.13	120.06	117.00
1	AA	780	A	C4-C5-C6	6.13	120.06	117.00
26	BA	705	A	N3-C4-N9	6.13	132.30	127.40
27	BB	29	A	C4-C5-C6	6.13	120.06	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1502	A	C4-C5-C6	6.13	120.06	117.00
26	BA	190	A	N3-C4-N9	6.13	132.30	127.40
26	BA	2378	A	C4-C5-C6	6.13	120.06	117.00
26	BA	2516	A	N3-C4-N9	6.13	132.30	127.40
1	AA	608	A	C4-C5-C6	6.13	120.06	117.00
26	BA	195	A	C4-C5-C6	6.13	120.06	117.00
26	BA	917	A	N3-C4-N9	6.13	132.30	127.40
1	AA	621	A	C4-C5-C6	6.12	120.06	117.00
1	AA	949	A	C4-C5-C6	6.12	120.06	117.00
26	BA	2386	A	C4-C5-C6	6.12	120.06	117.00
1	AA	53	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1318	A	C4-C5-C6	6.12	120.06	117.00
25	AY	23	A	C4-C5-C6	6.12	120.06	117.00
26	BA	794	A	N3-C4-N9	6.12	132.30	127.40
26	BA	2587	A	C4-C5-C6	6.12	120.06	117.00
26	BA	471	A	N3-C4-N9	6.12	132.30	127.40
26	BA	2856	A	C4-C5-C6	6.12	120.06	117.00
26	BA	1603	A	C4-C5-C6	6.12	120.06	117.00
26	BA	2518	A	N3-C4-N9	6.12	132.29	127.40
1	AA	642	A	C4-C5-C6	6.12	120.06	117.00
26	BA	730	A	C4-C5-C6	6.12	120.06	117.00
26	BA	1241	A	N3-C4-N9	6.12	132.29	127.40
26	BA	415	A	C4-C5-C6	6.12	120.06	117.00
26	BA	705	A	C4-C5-C6	6.12	120.06	117.00
26	BA	2657	A	C4-C5-C6	6.12	120.06	117.00
1	AA	938	A	C4-C5-C6	6.11	120.06	117.00
26	BA	1084	A	C4-C5-C6	6.11	120.06	117.00
27	BB	73	A	C4-C5-C6	6.11	120.06	117.00
26	BA	2516	A	C4-C5-C6	6.11	120.06	117.00
1	AA	901	A	N3-C4-N9	6.11	132.29	127.40
24	AX	23	A	C4-C5-C6	6.11	120.06	117.00
26	BA	1572	A	C4-C5-C6	6.11	120.06	117.00
26	BA	2725	A	N3-C4-N9	6.11	132.29	127.40
1	AA	1152	A	N3-C4-N9	6.11	132.29	127.40
26	BA	1287	A	C4-C5-C6	6.11	120.05	117.00
26	BA	2725	A	C4-C5-C6	6.11	120.06	117.00
1	AA	873	A	N3-C4-N9	6.11	132.28	127.40
26	BA	547	A	N3-C4-N9	6.11	132.28	127.40
1	AA	119	A	C4-C5-C6	6.11	120.05	117.00
26	BA	833	A	C4-C5-C6	6.11	120.05	117.00
26	BA	1088	A	C4-C5-C6	6.11	120.05	117.00
26	BA	2013	A	C4-C5-C6	6.11	120.05	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	55	A	N3-C4-N9	6.10	132.28	127.40
26	BA	152	A	C4-C5-C6	6.10	120.05	117.00
26	BA	374	A	C4-C5-C6	6.10	120.05	117.00
26	BA	449	A	N3-C4-N9	6.10	132.28	127.40
26	BA	1608	A	C4-C5-C6	6.10	120.05	117.00
26	BA	2800	A	C4-C5-C6	6.10	120.05	117.00
26	BA	2813	A	C4-C5-C6	6.10	120.05	117.00
25	AY	6	A	N3-C4-N9	6.10	132.28	127.40
26	BA	654	A	N3-C4-N9	6.10	132.28	127.40
26	BA	1244	A	N3-C4-N9	6.10	132.28	127.40
26	BA	1276	A	C4-C5-C6	6.10	120.05	117.00
26	BA	1579	A	C4-C5-C6	6.10	120.05	117.00
26	BA	2327	A	C4-C5-C6	6.10	120.05	117.00
1	AA	938	A	N3-C4-N9	6.10	132.28	127.40
23	AW	59	A	C4-C5-C6	6.10	120.05	117.00
25	AY	6	A	C4-C5-C6	6.10	120.05	117.00
26	BA	582	A	N3-C4-N9	6.10	132.28	127.40
26	BA	1919	A	N3-C4-N9	6.10	132.28	127.40
26	BA	1969	A	N3-C4-N9	6.10	132.28	127.40
1	AA	1357	A	N3-C4-N9	6.10	132.28	127.40
1	AA	1476	A	C4-C5-C6	6.10	120.05	117.00
24	AX	24	A	N3-C4-N9	6.10	132.28	127.40
1	AA	496	A	C4-C5-C6	6.09	120.05	117.00
1	AA	579	A	N3-C4-N9	6.09	132.28	127.40
25	AY	69	A	C4-C5-C6	6.09	120.05	117.00
26	BA	231	A	N3-C4-N9	6.09	132.28	127.40
26	BA	346	A	C4-C5-C6	6.09	120.05	117.00
26	BA	2531	A	C4-C5-C6	6.09	120.05	117.00
1	AA	1004	A	C4-C5-C6	6.09	120.05	117.00
26	BA	528	A	C4-C5-C6	6.09	120.05	117.00
26	BA	750	A	C4-C5-C6	6.09	120.05	117.00
26	BA	2191	A	C4-C5-C6	6.09	120.05	117.00
1	AA	496	A	N3-C4-N9	6.09	132.27	127.40
26	BA	131	A	C4-C5-C6	6.09	120.05	117.00
26	BA	1494	A	N3-C4-N9	6.09	132.27	127.40
26	BA	2163	A	N3-C4-N9	6.09	132.27	127.40
26	BA	2461	A	C4-C5-C6	6.09	120.05	117.00
27	BB	115	A	C4-C5-C6	6.09	120.05	117.00
1	AA	1306	A	C4-C5-C6	6.09	120.05	117.00
26	BA	1265	A	C8-N9-C4	6.09	108.24	105.80
26	BA	2837	A	C4-C5-C6	6.09	120.05	117.00
1	AA	502	A	C4-C5-C6	6.09	120.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1319	A	C4-C5-C6	6.09	120.04	117.00
26	BA	716	A	C4-C5-C6	6.09	120.04	117.00
1	AA	71	A	C4-C5-C6	6.09	120.04	117.00
26	BA	1762	A	C4-C5-C6	6.09	120.04	117.00
1	AA	389	A	N3-C4-N9	6.08	132.27	127.40
26	BA	1048	A	N3-C4-N9	6.08	132.27	127.40
26	BA	1549	A	C4-C5-C6	6.08	120.04	117.00
26	BA	2273	A	N3-C4-N9	6.08	132.27	127.40
1	AA	781	A	C4-C5-C6	6.08	120.04	117.00
26	BA	1143	A	C4-C5-C6	6.08	120.04	117.00
26	BA	1387	A	C4-C5-C6	6.08	120.04	117.00
27	BB	57	A	C4-C5-C6	6.08	120.04	117.00
26	BA	64	A	N3-C4-N9	6.08	132.26	127.40
26	BA	152	A	N3-C4-N9	6.08	132.26	127.40
26	BA	925	A	C4-C5-C6	6.08	120.04	117.00
26	BA	2054	A	N3-C4-N9	6.08	132.27	127.40
1	AA	1191	A	C4-C5-C6	6.08	120.04	117.00
26	BA	1086	A	N3-C4-N9	6.08	132.26	127.40
1	AA	468	A	N3-C4-N9	6.08	132.26	127.40
1	AA	1036	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1418	A	N3-C4-N9	6.08	132.26	127.40
1	AA	1430	A	C4-C5-C6	6.08	120.04	117.00
24	AX	23	A	N3-C4-N9	6.08	132.26	127.40
26	BA	402	A	C4-C5-C6	6.08	120.04	117.00
26	BA	820	A	N3-C4-N9	6.08	132.26	127.40
26	BA	2080	A	N3-C4-N9	6.08	132.26	127.40
26	BA	472	A	C4-C5-C6	6.08	120.04	117.00
26	BA	693	A	C4-C5-C6	6.08	120.04	117.00
26	BA	715	A	C4-C5-C6	6.08	120.04	117.00
1	AA	28	A	C4-C5-C6	6.08	120.04	117.00
1	AA	595	A	C4-C5-C6	6.08	120.04	117.00
1	AA	621	A	N3-C4-N9	6.08	132.26	127.40
26	BA	706	A	N3-C4-N9	6.08	132.26	127.40
26	BA	1791	A	C4-C5-C6	6.08	120.04	117.00
26	BA	2392	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1324	A	C4-C5-C6	6.07	120.04	117.00
26	BA	101	A	C4-C5-C6	6.07	120.04	117.00
26	BA	975	A	C4-C5-C6	6.07	120.04	117.00
26	BA	2015	A	C4-C5-C6	6.07	120.04	117.00
1	AA	908	A	N3-C4-N9	6.07	132.26	127.40
26	BA	1773	A	C4-C5-C6	6.07	120.04	117.00
26	BA	1927	A	C4-C5-C6	6.07	120.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	373	A	N3-C4-N9	6.07	132.26	127.40
1	AA	1219	A	C4-C5-C6	6.07	120.03	117.00
26	BA	428	A	C4-C5-C6	6.07	120.03	117.00
26	BA	756	A	N3-C4-N9	6.07	132.26	127.40
26	BA	1048	A	C4-C5-C6	6.07	120.03	117.00
26	BA	1532	A	C4-C5-C6	6.07	120.04	117.00
1	AA	923	A	N3-C4-N9	6.07	132.25	127.40
1	AA	1022	A	C4-C5-C6	6.07	120.03	117.00
26	BA	1745	A	C4-C5-C6	6.07	120.03	117.00
26	BA	2873	A	C4-C5-C6	6.07	120.03	117.00
27	BB	15	A	C4-C5-C6	6.07	120.03	117.00
1	AA	1022	A	N3-C4-N9	6.07	132.25	127.40
23	AW	58	A	C4-C5-C6	6.07	120.03	117.00
26	BA	1548	A	C4-C5-C6	6.07	120.03	117.00
26	BA	2518	A	C4-C5-C6	6.07	120.03	117.00
1	AA	640	A	N3-C4-N9	6.07	132.25	127.40
26	BA	423	A	C4-C5-C6	6.07	120.03	117.00
1	AA	262	A	C4-C5-C6	6.06	120.03	117.00
1	AA	460	A	C4-C5-C6	6.06	120.03	117.00
1	AA	1080	A	C4-C5-C6	6.06	120.03	117.00
26	BA	1169	A	C4-C5-C6	6.06	120.03	117.00
26	BA	1784	A	C4-C5-C6	6.06	120.03	117.00
26	BA	2311	A	N3-C4-N9	6.06	132.25	127.40
1	AA	55	A	C4-C5-C6	6.06	120.03	117.00
1	AA	192	A	C4-C5-C6	6.06	120.03	117.00
1	AA	468	A	C4-C5-C6	6.06	120.03	117.00
26	BA	1470	A	C4-C5-C6	6.06	120.03	117.00
1	AA	448	A	N3-C4-N9	6.06	132.25	127.40
1	AA	1252	A	C4-C5-C6	6.06	120.03	117.00
26	BA	362	A	C4-C5-C6	6.06	120.03	117.00
26	BA	454	A	C4-C5-C6	6.06	120.03	117.00
26	BA	677	A	C8-N9-C4	6.06	108.22	105.80
26	BA	2471	A	C4-C5-C6	6.06	120.03	117.00
1	AA	743	A	N3-C4-N9	6.06	132.25	127.40
1	AA	1021	A	C4-C5-C6	6.06	120.03	117.00
1	AA	1396	A	C4-C5-C6	6.06	120.03	117.00
23	AW	26	A	C4-C5-C6	6.06	120.03	117.00
23	AW	26	A	N3-C4-N9	6.06	132.25	127.40
26	BA	1127	A	C4-C5-C6	6.06	120.03	117.00
26	BA	1433	A	C4-C5-C6	6.06	120.03	117.00
1	AA	59	A	C4-C5-C6	6.06	120.03	117.00
1	AA	263	A	C4-C5-C6	6.06	120.03	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	794	A	C4-C5-C6	6.06	120.03	117.00
1	AA	1152	A	C4-C5-C6	6.06	120.03	117.00
26	BA	182	A	C4-C5-C6	6.06	120.03	117.00
26	BA	654	A	C4-C5-C6	6.06	120.03	117.00
26	BA	2317	A	C4-C5-C6	6.06	120.03	117.00
26	BA	2439	A	C4-C5-C6	6.06	120.03	117.00
1	AA	600	A	C4-C5-C6	6.06	120.03	117.00
26	BA	131	A	N3-C4-N9	6.06	132.24	127.40
26	BA	501	A	C4-C5-C6	6.06	120.03	117.00
26	BA	1591	A	C4-C5-C6	6.06	120.03	117.00
26	BA	2879	A	C4-C5-C6	6.06	120.03	117.00
1	AA	1429	A	N3-C4-N9	6.05	132.24	127.40
26	BA	299	A	C4-C5-C6	6.05	120.03	117.00
26	BA	1810	A	N3-C4-N9	6.05	132.24	127.40
26	BA	2212	A	C4-C5-C6	6.05	120.03	117.00
26	BA	2675	A	C4-C5-C6	6.05	120.03	117.00
26	BA	2823	A	C4-C5-C6	6.05	120.03	117.00
27	BB	53	A	C4-C5-C6	6.05	120.03	117.00
1	AA	865	A	C4-C5-C6	6.05	120.03	117.00
1	AA	553	A	C4-C5-C6	6.05	120.03	117.00
26	BA	173	A	N3-C4-N9	6.05	132.24	127.40
26	BA	959	A	C4-C5-C6	6.05	120.03	117.00
26	BA	1618	A	C4-C5-C6	6.05	120.03	117.00
26	BA	2386	A	N3-C4-N9	6.05	132.24	127.40
1	AA	906	A	C4-C5-C6	6.05	120.03	117.00
1	AA	1476	A	N3-C4-N9	6.05	132.24	127.40
26	BA	191	A	N3-C4-N9	6.05	132.24	127.40
26	BA	1247	A	C4-C5-C6	6.05	120.03	117.00
26	BA	1307	A	C4-C5-C6	6.05	120.03	117.00
26	BA	1496	A	C4-C5-C6	6.05	120.02	117.00
26	BA	1525	A	C4-C5-C6	6.05	120.02	117.00
26	BA	2635	A	C4-C5-C6	6.05	120.03	117.00
1	AA	33	A	C4-C5-C6	6.05	120.02	117.00
26	BA	735	A	C4-C5-C6	6.05	120.02	117.00
24	AX	24	A	C4-C5-C6	6.05	120.02	117.00
26	BA	1353	A	N3-C4-N9	6.05	132.24	127.40
26	BA	2598	A	C4-C5-C6	6.05	120.02	117.00
26	BA	547	A	C4-C5-C6	6.04	120.02	117.00
26	BA	2094	A	C4-C5-C6	6.04	120.02	117.00
1	AA	306	A	C4-C5-C6	6.04	120.02	117.00
1	AA	918	A	N3-C4-N9	6.04	132.23	127.40
1	AA	1329	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	AV	17	A	C4-C5-C6	6.04	120.02	117.00
26	BA	94	A	C4-C5-C6	6.04	120.02	117.00
26	BA	1089	A	C4-C5-C6	6.04	120.02	117.00
26	BA	1095	A	C4-C5-C6	6.04	120.02	117.00
26	BA	1269	A	C4-C5-C6	6.04	120.02	117.00
26	BA	1634	A	N3-C4-N9	6.04	132.23	127.40
26	BA	1676	A	C4-C5-C6	6.04	120.02	117.00
26	BA	2173	A	C4-C5-C6	6.04	120.02	117.00
26	BA	2531	A	N3-C4-N9	6.04	132.24	127.40
26	BA	2634	A	C4-C5-C6	6.04	120.02	117.00
1	AA	482	A	N3-C4-N9	6.04	132.23	127.40
1	AA	495	A	N3-C4-N9	6.04	132.23	127.40
1	AA	1014	A	C4-C5-C6	6.04	120.02	117.00
1	AA	1035	A	C4-C5-C6	6.04	120.02	117.00
26	BA	282	A	C4-C5-C6	6.04	120.02	117.00
26	BA	722	A	C4-C5-C6	6.04	120.02	117.00
26	BA	1528	A	C4-C5-C6	6.04	120.02	117.00
26	BA	1977	A	C4-C5-C6	6.04	120.02	117.00
26	BA	2657	A	N3-C4-N9	6.04	132.23	127.40
1	AA	300	A	N3-C4-N9	6.04	132.23	127.40
1	AA	344	A	C4-C5-C6	6.04	120.02	117.00
1	AA	1340	A	C4-C5-C6	6.04	120.02	117.00
1	AA	1531	A	C4-C5-C6	6.04	120.02	117.00
26	BA	1365	A	C4-C5-C6	6.04	120.02	117.00
1	AA	441	A	C8-N9-C4	6.04	108.22	105.80
1	AA	753	A	C4-C5-C6	6.04	120.02	117.00
1	AA	1332	A	N3-C4-N9	6.04	132.23	127.40
26	BA	1809	A	C4-C5-C6	6.04	120.02	117.00
1	AA	630	A	C4-C5-C6	6.04	120.02	117.00
1	AA	746	A	N3-C4-N9	6.04	132.23	127.40
1	AA	1176	A	C4-C5-C6	6.04	120.02	117.00
26	BA	1496	A	N3-C4-N9	6.04	132.23	127.40
1	AA	845	A	C4-C5-C6	6.04	120.02	117.00
1	AA	1180	A	C4-C5-C6	6.04	120.02	117.00
26	BA	541	A	C4-C5-C6	6.04	120.02	117.00
26	BA	1387	A	N3-C4-N9	6.04	132.23	127.40
26	BA	1901	A	N3-C4-N9	6.04	132.23	127.40
26	BA	2088	A	N3-C4-N9	6.04	132.23	127.40
26	BA	2850	A	C4-C5-C6	6.04	120.02	117.00
1	AA	1360	A	C4-C5-C6	6.03	120.02	117.00
26	BA	613	A	C4-C5-C6	6.03	120.02	117.00
26	BA	1133	A	C4-C5-C6	6.03	120.02	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1502	A	C4-C5-C6	6.03	120.02	117.00
26	BA	1928	A	C4-C5-C6	6.03	120.02	117.00
26	BA	1936	A	C4-C5-C6	6.03	120.02	117.00
1	AA	32	A	C4-C5-C6	6.03	120.02	117.00
25	AY	66	A	N3-C4-N9	6.03	132.22	127.40
26	BA	10	A	N3-C4-N9	6.03	132.22	127.40
26	BA	1634	A	C8-N9-C4	6.03	108.21	105.80
26	BA	1998	A	C4-C5-C6	6.03	120.02	117.00
1	AA	1493	A	N9-C4-C5	6.03	108.21	105.80
24	AX	3	A	C4-C5-C6	6.03	120.02	117.00
26	BA	348	A	C4-C5-C6	6.03	120.01	117.00
26	BA	984	A	C4-C5-C6	6.03	120.02	117.00
26	BA	1698	A	C4-C5-C6	6.03	120.02	117.00
26	BA	2778	A	N3-C4-N9	6.03	132.22	127.40
26	BA	160	A	N3-C4-N9	6.03	132.22	127.40
26	BA	522	A	C4-C5-C6	6.03	120.01	117.00
26	BA	718	A	C4-C5-C6	6.03	120.01	117.00
26	BA	1504	A	C4-C5-C6	6.03	120.01	117.00
26	BA	1679	A	C4-C5-C6	6.03	120.01	117.00
26	BA	2088	A	C4-C5-C6	6.03	120.01	117.00
26	BA	2191	A	N3-C4-N9	6.03	132.22	127.40
1	AA	205	A	C4-C5-C6	6.03	120.01	117.00
23	AW	38	A	C4-C5-C6	6.03	120.01	117.00
24	AX	19	U	C6-N1-C2	6.03	124.61	121.00
26	BA	670	A	C4-C5-C6	6.03	120.01	117.00
26	BA	792	A	C4-C5-C6	6.03	120.01	117.00
26	BA	1287	A	N3-C4-N9	6.03	132.22	127.40
26	BA	1504	A	N3-C4-N9	6.03	132.22	127.40
26	BA	1847	A	C4-C5-C6	6.03	120.01	117.00
26	BA	2184	A	N3-C4-N9	6.03	132.22	127.40
25	AY	21	A	C4-C5-C6	6.02	120.01	117.00
26	BA	752	A	C4-C5-C6	6.02	120.01	117.00
26	BA	1365	A	N3-C4-N9	6.02	132.22	127.40
1	AA	1239	A	C8-N9-C4	6.02	108.21	105.80
26	BA	10	A	C4-C5-C6	6.02	120.01	117.00
26	BA	457	A	C8-N9-C4	6.02	108.21	105.80
26	BA	739	A	C4-C5-C6	6.02	120.01	117.00
26	BA	751	A	C4-C5-C6	6.02	120.01	117.00
26	BA	1039	A	C4-C5-C6	6.02	120.01	117.00
26	BA	1151	A	C4-C5-C6	6.02	120.01	117.00
26	BA	1548	A	N3-C4-N9	6.02	132.22	127.40
26	BA	1641	A	C4-C5-C6	6.02	120.01	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2051	A	N3-C4-N9	6.02	132.22	127.40
26	BA	2328	A	N3-C4-N9	6.02	132.22	127.40
26	BA	1858	A	C4-C5-C6	6.02	120.01	117.00
27	BB	78	A	N9-C4-C5	6.02	108.21	105.80
1	AA	1429	A	C4-C5-C6	6.02	120.01	117.00
26	BA	2205	A	C4-C5-C6	6.02	120.01	117.00
26	BA	2733	A	C4-C5-C6	6.02	120.01	117.00
27	BB	45	A	C4-C5-C6	6.02	120.01	117.00
27	BB	57	A	N3-C4-N9	6.02	132.22	127.40
1	AA	373	A	C4-C5-C6	6.02	120.01	117.00
26	BA	279	A	N3-C4-N9	6.02	132.22	127.40
26	BA	422	A	C4-C5-C6	6.02	120.01	117.00
26	BA	877	A	C4-C5-C6	6.02	120.01	117.00
26	BA	1027	A	C4-C5-C6	6.02	120.01	117.00
26	BA	1453	A	C4-C5-C6	6.02	120.01	117.00
26	BA	2095	A	C4-C5-C6	6.02	120.01	117.00
26	BA	2542	A	C8-N9-C4	6.02	108.21	105.80
26	BA	2740	A	C4-C5-C6	6.02	120.01	117.00
26	BA	2879	A	N3-C4-N9	6.02	132.21	127.40
1	AA	189	A	C4-C5-C6	6.02	120.01	117.00
1	AA	1261	A	N3-C4-N9	6.02	132.21	127.40
26	BA	382	A	C4-C5-C6	6.02	120.01	117.00
1	AA	236	A	C4-C5-C6	6.01	120.01	117.00
1	AA	502	A	N3-C4-N9	6.01	132.21	127.40
1	AA	1171	A	C4-C5-C6	6.01	120.01	117.00
1	AA	1269	A	C4-C5-C6	6.01	120.01	117.00
1	AA	1503	A	C4-C5-C6	6.01	120.01	117.00
26	BA	219	A	C4-C5-C6	6.01	120.01	117.00
26	BA	563	A	C4-C5-C6	6.01	120.01	117.00
26	BA	1566	A	C4-C5-C6	6.01	120.01	117.00
26	BA	1744	A	C4-C5-C6	6.01	120.01	117.00
26	BA	2727	A	N3-C4-N9	6.01	132.21	127.40
1	AA	892	A	C4-C5-C6	6.01	120.01	117.00
24	AX	14	A	C4-C5-C6	6.01	120.01	117.00
24	AX	14	A	N3-C4-N9	6.01	132.21	127.40
26	BA	800	A	C8-N9-C4	6.01	108.20	105.80
26	BA	2013	A	N3-C4-N9	6.01	132.21	127.40
26	BA	2433	A	C4-C5-C6	6.01	120.01	117.00
26	BA	2778	A	C4-C5-C6	6.01	120.01	117.00
1	AA	414	A	C4-C5-C6	6.01	120.01	117.00
1	AA	1339	A	N3-C4-N9	6.01	132.21	127.40
1	AA	1508	A	C4-C5-C6	6.01	120.01	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AV	20	A	C4-C5-C6	6.01	120.00	117.00
23	AW	20	U	C6-N1-C2	6.01	124.61	121.00
23	AW	73	A	C4-C5-C6	6.01	120.01	117.00
26	BA	176	A	N3-C4-N9	6.01	132.21	127.40
26	BA	251	A	N3-C4-N9	6.01	132.21	127.40
26	BA	391	A	N3-C4-N9	6.01	132.21	127.40
26	BA	1268	A	C4-C5-C6	6.01	120.01	117.00
1	AA	32	A	N3-C4-N9	6.01	132.21	127.40
1	AA	510	A	C4-C5-C6	6.01	120.00	117.00
1	AA	900	A	C4-C5-C6	6.01	120.00	117.00
1	AA	1519	A	C4-C5-C6	6.01	120.00	117.00
26	BA	556	A	C4-C5-C6	6.01	120.00	117.00
26	BA	1226	A	C4-C5-C6	6.01	120.00	117.00
26	BA	1981	A	C4-C5-C6	6.01	120.00	117.00
26	BA	2900	A	C4-C5-C6	6.01	120.00	117.00
1	AA	831	A	C4-C5-C6	6.01	120.00	117.00
24	AX	20	U	C6-N1-C2	6.01	124.61	121.00
26	BA	1912	A	C4-C5-C6	6.01	120.00	117.00
26	BA	2042	A	C4-C5-C6	6.01	120.00	117.00
26	BA	2471	A	N3-C4-N9	6.01	132.21	127.40
1	AA	109	A	C4-C5-C6	6.01	120.00	117.00
1	AA	702	A	C4-C5-C6	6.01	120.00	117.00
1	AA	1499	A	C4-C5-C6	6.01	120.00	117.00
23	AW	59	A	N3-C4-N9	6.01	132.20	127.40
26	BA	14	A	C4-C5-C6	6.01	120.00	117.00
26	BA	21	A	C4-C5-C6	6.01	120.00	117.00
26	BA	119	A	N9-C4-C5	6.01	108.20	105.80
26	BA	789	A	C4-C5-C6	6.01	120.00	117.00
26	BA	1392	A	C4-C5-C6	6.01	120.00	117.00
26	BA	1603	A	N3-C4-N9	6.01	132.21	127.40
26	BA	1635	A	C4-C5-C6	6.01	120.00	117.00
26	BA	1735	A	C4-C5-C6	6.01	120.00	117.00
26	BA	2060	A	C4-C5-C6	6.01	120.00	117.00
26	BA	2184	A	C4-C5-C6	6.01	120.00	117.00
1	AA	746	A	C4-C5-C6	6.00	120.00	117.00
26	BA	197	A	N3-C4-N9	6.00	132.20	127.40
26	BA	2094	A	N3-C4-N9	6.00	132.20	127.40
26	BA	2352	A	N3-C4-N9	6.00	132.20	127.40
1	AA	787	A	C4-C5-C6	6.00	120.00	117.00
1	AA	935	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1350	A	C4-C5-C6	6.00	120.00	117.00
26	BA	443	A	C4-C5-C6	6.00	120.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1111	A	C4-C5-C6	6.00	120.00	117.00
26	BA	1385	A	C8-N9-C4	6.00	108.20	105.80
26	BA	1508	A	C4-C5-C6	6.00	120.00	117.00
26	BA	1571	A	N3-C4-N9	6.00	132.20	127.40
26	BA	1744	A	N3-C4-N9	6.00	132.20	127.40
26	BA	2459	A	C4-C5-C6	6.00	120.00	117.00
26	BA	2758	A	C4-C5-C6	6.00	120.00	117.00
1	AA	8	A	C8-N9-C4	6.00	108.20	105.80
1	AA	149	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1362	A	N3-C4-N9	6.00	132.20	127.40
26	BA	1046	A	N3-C4-N9	6.00	132.20	127.40
26	BA	1637	A	C4-C5-C6	6.00	120.00	117.00
26	BA	1848	A	C4-C5-C6	6.00	120.00	117.00
26	BA	2439	A	N3-C4-N9	6.00	132.20	127.40
26	BA	1264	A	C4-C5-C6	6.00	120.00	117.00
26	BA	1469	A	N3-C4-N9	6.00	132.20	127.40
26	BA	1608	A	N3-C4-N9	6.00	132.20	127.40
1	AA	71	A	N3-C4-N9	6.00	132.20	127.40
1	AA	303	A	C4-C5-C6	6.00	120.00	117.00
1	AA	716	A	C4-C5-C6	6.00	120.00	117.00
1	AA	864	A	N3-C4-N9	6.00	132.20	127.40
1	AA	968	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1271	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1349	A	C4-C5-C6	6.00	120.00	117.00
26	BA	432	A	C4-C5-C6	6.00	120.00	117.00
26	BA	602	A	C4-C5-C6	6.00	120.00	117.00
26	BA	866	A	C4-C5-C6	6.00	120.00	117.00
26	BA	1434	A	C4-C5-C6	6.00	120.00	117.00
26	BA	1877	A	C4-C5-C6	6.00	120.00	117.00
26	BA	1899	A	N3-C4-N9	6.00	132.20	127.40
26	BA	2014	A	N3-C4-N9	6.00	132.20	127.40
26	BA	2376	A	C4-C5-C6	6.00	120.00	117.00
1	AA	53	A	N3-C4-N9	6.00	132.20	127.40
1	AA	306	A	N3-C4-N9	6.00	132.20	127.40
1	AA	451	A	N3-C4-N9	6.00	132.20	127.40
1	AA	1465	A	C4-C5-C6	6.00	120.00	117.00
26	BA	374	A	N3-C4-N9	6.00	132.20	127.40
26	BA	804	A	C4-C5-C6	6.00	120.00	117.00
26	BA	825	A	C4-C5-C6	6.00	120.00	117.00
26	BA	1745	A	N3-C4-N9	6.00	132.20	127.40
26	BA	2336	A	C4-C5-C6	6.00	120.00	117.00
26	BA	2809	A	C4-C5-C6	6.00	120.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2856	A	N3-C4-N9	6.00	132.20	127.40
26	BA	2886	A	C4-C5-C6	6.00	120.00	117.00
1	AA	728	A	C4-C5-C6	6.00	120.00	117.00
26	BA	173	A	C4-C5-C6	6.00	120.00	117.00
26	BA	1505	A	C4-C5-C6	6.00	120.00	117.00
26	BA	2468	A	C4-C5-C6	6.00	120.00	117.00
26	BA	2837	A	N3-C4-N9	6.00	132.20	127.40
1	AA	435	A	N3-C4-N9	5.99	132.19	127.40
1	AA	696	A	C4-C5-C6	5.99	120.00	117.00
1	AA	1236	A	C4-C5-C6	5.99	120.00	117.00
26	BA	439	A	C4-C5-C6	5.99	120.00	117.00
26	BA	1189	A	C4-C5-C6	5.99	120.00	117.00
26	BA	1495	A	C4-C5-C6	5.99	120.00	117.00
1	AA	152	A	C4-C5-C6	5.99	120.00	117.00
26	BA	2776	A	N3-C4-N9	5.99	132.19	127.40
26	BA	2792	A	C4-C5-C6	5.99	120.00	117.00
1	AA	51	A	C4-C5-C6	5.99	120.00	117.00
1	AA	81	A	C4-C5-C6	5.99	120.00	117.00
1	AA	228	A	C4-C5-C6	5.99	120.00	117.00
1	AA	864	A	C4-C5-C6	5.99	120.00	117.00
1	AA	1377	A	C4-C5-C6	5.99	120.00	117.00
24	AX	21	A	C4-C5-C6	5.99	120.00	117.00
26	BA	1000	A	N3-C4-N9	5.99	132.19	127.40
26	BA	1328	A	C4-C5-C6	5.99	120.00	117.00
26	BA	1354	A	C4-C5-C6	5.99	120.00	117.00
26	BA	1783	A	C4-C5-C6	5.99	120.00	117.00
26	BA	2887	A	N3-C4-N9	5.99	132.19	127.40
1	AA	958	A	C4-C5-C6	5.99	120.00	117.00
1	AA	1188	A	C4-C5-C6	5.99	119.99	117.00
26	BA	415	A	N3-C4-N9	5.99	132.19	127.40
26	BA	2577	A	C4-C5-C6	5.99	120.00	117.00
26	BA	2711	A	C4-C5-C6	5.99	120.00	117.00
26	BA	13	A	C4-C5-C6	5.99	119.99	117.00
26	BA	73	A	C4-C5-C6	5.99	119.99	117.00
26	BA	218	A	C4-C5-C6	5.99	119.99	117.00
26	BA	294	A	C4-C5-C6	5.99	119.99	117.00
26	BA	332	A	C4-C5-C6	5.99	119.99	117.00
26	BA	1189	A	N3-C4-N9	5.99	132.19	127.40
26	BA	2333	A	N3-C4-N9	5.99	132.19	127.40
26	BA	2860	A	C4-C5-C6	5.99	119.99	117.00
1	AA	19	A	C4-C5-C6	5.99	119.99	117.00
26	BA	161	A	C4-C5-C6	5.99	119.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	352	A	N3-C4-N9	5.99	132.19	127.40
26	BA	429	A	C4-C5-C6	5.99	119.99	117.00
26	BA	1274	A	C4-C5-C6	5.99	119.99	117.00
26	BA	1654	A	C4-C5-C6	5.99	119.99	117.00
26	BA	1952	A	C4-C5-C6	5.99	119.99	117.00
26	BA	2336	A	N3-C4-N9	5.99	132.19	127.40
26	BA	2654	A	C4-C5-C6	5.99	119.99	117.00
26	BA	2706	A	C4-C5-C6	5.99	119.99	117.00
1	AA	60	A	C8-N9-C4	5.98	108.19	105.80
26	BA	1262	A	N3-C4-N9	5.98	132.19	127.40
26	BA	1367	A	C4-C5-C6	5.98	119.99	117.00
26	BA	2169	A	N3-C4-N9	5.98	132.19	127.40
1	AA	607	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1163	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1433	A	C4-C5-C6	5.98	119.99	117.00
22	AV	19	A	C4-C5-C6	5.98	119.99	117.00
24	AX	16	U	C6-N1-C2	5.98	124.59	121.00
26	BA	63	A	C4-C5-C6	5.98	119.99	117.00
26	BA	391	A	C4-C5-C6	5.98	119.99	117.00
26	BA	928	A	C4-C5-C6	5.98	119.99	117.00
26	BA	1103	A	N3-C4-N9	5.98	132.19	127.40
26	BA	1144	A	C4-C5-C6	5.98	119.99	117.00
26	BA	1439	A	C4-C5-C6	5.98	119.99	117.00
26	BA	1549	A	N3-C4-N9	5.98	132.19	127.40
26	BA	1632	A	C4-C5-C6	5.98	119.99	117.00
26	BA	2333	A	C4-C5-C6	5.98	119.99	117.00
26	BA	2432	A	C4-C5-C6	5.98	119.99	117.00
26	BA	2700	A	C4-C5-C6	5.98	119.99	117.00
26	BA	2810	A	C4-C5-C6	5.98	119.99	117.00
1	AA	353	A	N3-C4-N9	5.98	132.18	127.40
1	AA	573	A	C4-C5-C6	5.98	119.99	117.00
1	AA	607	A	N3-C4-N9	5.98	132.18	127.40
1	AA	1483	A	N3-C4-N9	5.98	132.19	127.40
26	BA	111	A	C4-C5-C6	5.98	119.99	117.00
26	BA	127	A	C4-C5-C6	5.98	119.99	117.00
26	BA	233	A	N3-C4-N9	5.98	132.18	127.40
26	BA	447	A	N3-C4-N9	5.98	132.19	127.40
26	BA	1050	A	C4-C5-C6	5.98	119.99	117.00
26	BA	1086	A	C4-C5-C6	5.98	119.99	117.00
26	BA	1175	A	C4-C5-C6	5.98	119.99	117.00
26	BA	1327	A	C4-C5-C6	5.98	119.99	117.00
26	BA	1373	A	C4-C5-C6	5.98	119.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1676	A	N3-C4-N9	5.98	132.19	127.40
26	BA	1872	A	C4-C5-C6	5.98	119.99	117.00
26	BA	2366	A	N3-C4-N9	5.98	132.18	127.40
1	AA	192	A	N3-C4-N9	5.98	132.18	127.40
1	AA	1261	A	C4-C5-C6	5.98	119.99	117.00
24	AX	3	A	N3-C4-N9	5.98	132.18	127.40
26	BA	743	A	C4-C5-C6	5.98	119.99	117.00
26	BA	1591	A	N3-C4-N9	5.98	132.18	127.40
26	BA	2020	A	C4-C5-C6	5.98	119.99	117.00
26	BA	2740	A	N3-C4-N9	5.98	132.18	127.40
27	BB	109	A	C4-C5-C6	5.98	119.99	117.00
1	AA	129	A	C4-C5-C6	5.98	119.99	117.00
1	AA	151	A	N9-C4-C5	5.98	108.19	105.80
1	AA	523	A	C4-C5-C6	5.98	119.99	117.00
1	AA	825	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1256	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1318	A	N3-C4-N9	5.98	132.18	127.40
1	AA	1396	A	N3-C4-N9	5.98	132.18	127.40
26	BA	28	A	C4-C5-C6	5.98	119.99	117.00
26	BA	103	A	N3-C4-N9	5.98	132.18	127.40
26	BA	345	A	C4-C5-C6	5.98	119.99	117.00
26	BA	1711	A	C4-C5-C6	5.98	119.99	117.00
26	BA	2082	A	N3-C4-N9	5.98	132.18	127.40
26	BA	2412	A	N3-C4-N9	5.98	132.18	127.40
26	BA	1169	A	N3-C4-N9	5.98	132.18	127.40
26	BA	1598	A	C4-C5-C6	5.98	119.99	117.00
26	BA	2309	A	C4-C5-C6	5.98	119.99	117.00
1	AA	74	A	C4-C5-N7	-5.97	107.71	110.70
1	AA	174	A	C4-C5-C6	5.97	119.99	117.00
1	AA	596	A	C4-C5-C6	5.97	119.99	117.00
1	AA	865	A	N3-C4-N9	5.97	132.18	127.40
1	AA	1446	A	C4-C5-C6	5.97	119.99	117.00
26	BA	734	A	C4-C5-C6	5.97	119.99	117.00
26	BA	829	A	C4-C5-C6	5.97	119.99	117.00
26	BA	1253	A	C4-C5-C6	5.97	119.99	117.00
26	BA	1477	A	C4-C5-C6	5.97	119.99	117.00
26	BA	2097	A	C4-C5-C6	5.97	119.99	117.00
26	BA	2706	A	N3-C4-N9	5.97	132.18	127.40
1	AA	431	A	C4-C5-C6	5.97	119.99	117.00
1	AA	968	A	N3-C4-N9	5.97	132.18	127.40
1	AA	1324	A	N3-C4-N9	5.97	132.18	127.40
1	AA	1394	A	C4-C5-C6	5.97	119.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	26	A	N3-C4-N9	5.97	132.18	127.40
26	BA	6	A	C4-C5-C6	5.97	119.99	117.00
26	BA	74	A	N3-C4-N9	5.97	132.18	127.40
26	BA	730	A	N3-C4-N9	5.97	132.18	127.40
26	BA	943	A	C4-C5-C6	5.97	119.99	117.00
26	BA	1085	A	C4-C5-C6	5.97	119.99	117.00
26	BA	1453	A	N3-C4-N9	5.97	132.18	127.40
1	AA	298	A	C4-C5-C6	5.97	119.98	117.00
1	AA	371	A	C4-C5-C6	5.97	119.98	117.00
1	AA	466	A	C4-C5-C6	5.97	119.98	117.00
26	BA	482	A	C4-C5-C6	5.97	119.98	117.00
26	BA	515	A	C4-C5-C6	5.97	119.98	117.00
26	BA	972	A	C4-C5-C6	5.97	119.98	117.00
26	BA	1889	A	C4-C5-C6	5.97	119.98	117.00
26	BA	2170	A	C4-C5-C6	5.97	119.98	117.00
26	BA	2758	A	N3-C4-N9	5.97	132.18	127.40
22	AV	20	A	N3-C4-N9	5.97	132.18	127.40
26	BA	466	A	C4-C5-C6	5.97	119.98	117.00
26	BA	2158	A	N3-C4-N9	5.97	132.17	127.40
26	BA	2602	A	C4-C5-C6	5.97	119.98	117.00
1	AA	238	A	C4-C5-C6	5.97	119.98	117.00
1	AA	452	A	N9-C4-C5	5.97	108.19	105.80
1	AA	675	A	C4-C5-C6	5.97	119.98	117.00
1	AA	784	A	C4-C5-C6	5.97	119.98	117.00
1	AA	935	A	N3-C4-N9	5.97	132.17	127.40
1	AA	1431	A	C4-C5-C6	5.97	119.98	117.00
25	AY	69	A	N3-C4-N9	5.97	132.17	127.40
26	BA	103	A	C4-C5-C6	5.97	119.98	117.00
26	BA	479	A	C4-C5-N7	-5.97	107.72	110.70
26	BA	988	A	C4-C5-C6	5.97	119.98	117.00
26	BA	1144	A	N3-C4-N9	5.97	132.17	127.40
26	BA	1327	A	N3-C4-N9	5.97	132.17	127.40
26	BA	2587	A	N3-C4-N9	5.97	132.17	127.40
1	AA	363	A	C4-C5-C6	5.96	119.98	117.00
1	AA	431	A	C4-C5-N7	-5.96	107.72	110.70
1	AA	1012	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1021	A	N3-C4-N9	5.96	132.17	127.40
1	AA	1499	A	N3-C4-N9	5.96	132.17	127.40
22	AV	19	A	N3-C4-N9	5.96	132.17	127.40
26	BA	347	A	C4-C5-C6	5.96	119.98	117.00
26	BA	514	A	N3-C4-N9	5.96	132.17	127.40
26	BA	892	A	C4-C5-C6	5.96	119.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1090	A	N3-C4-N9	5.96	132.17	127.40
26	BA	1272	A	C4-C5-C6	5.96	119.98	117.00
26	BA	1403	A	C4-C5-C6	5.96	119.98	117.00
26	BA	2054	A	C4-C5-C6	5.96	119.98	117.00
26	BA	2095	A	N3-C4-N9	5.96	132.17	127.40
26	BA	2476	A	N3-C4-N9	5.96	132.17	127.40
26	BA	2900	A	N3-C4-N9	5.96	132.17	127.40
27	BB	53	A	N3-C4-N9	5.96	132.17	127.40
26	BA	227	A	N3-C4-N9	5.96	132.17	127.40
26	BA	575	A	C4-C5-C6	5.96	119.98	117.00
26	BA	996	A	C4-C5-C6	5.96	119.98	117.00
26	BA	2142	A	C4-C5-C6	5.96	119.98	117.00
26	BA	2346	A	C4-C5-C6	5.96	119.98	117.00
26	BA	2497	A	C4-C5-C6	5.96	119.98	117.00
1	AA	704	A	C4-C5-C6	5.96	119.98	117.00
1	AA	777	A	C4-C5-C6	5.96	119.98	117.00
1	AA	816	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1081	A	C4-C5-C6	5.96	119.98	117.00
26	BA	165	A	C4-C5-C6	5.96	119.98	117.00
26	BA	256	A	N3-C4-N9	5.96	132.17	127.40
26	BA	346	A	N3-C4-N9	5.96	132.17	127.40
26	BA	430	A	C4-C5-C6	5.96	119.98	117.00
26	BA	453	A	C4-C5-C6	5.96	119.98	117.00
26	BA	504	A	C4-C5-C6	5.96	119.98	117.00
26	BA	505	A	C4-C5-C6	5.96	119.98	117.00
26	BA	1383	A	C4-C5-C6	5.96	119.98	117.00
26	BA	2327	A	N3-C4-N9	5.96	132.17	127.40
25	AY	23	A	N3-C4-N9	5.96	132.17	127.40
26	BA	2058	A	C4-C5-C6	5.96	119.98	117.00
1	AA	33	A	N3-C4-N9	5.96	132.17	127.40
1	AA	676	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1093	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1346	A	N3-C4-N9	5.96	132.17	127.40
23	AW	76	A	C4-C5-C6	5.96	119.98	117.00
24	AX	41	A	N3-C4-N9	5.96	132.17	127.40
26	BA	203	A	C4-C5-C6	5.96	119.98	117.00
26	BA	382	A	N3-C4-N9	5.96	132.17	127.40
26	BA	743	A	N3-C4-N9	5.96	132.17	127.40
26	BA	920	A	C4-C5-C6	5.96	119.98	117.00
26	BA	1470	A	N3-C4-N9	5.96	132.17	127.40
26	BA	1722	A	C4-C5-C6	5.96	119.98	117.00
26	BA	2406	A	C4-C5-C6	5.96	119.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	629	A	C4-C5-C6	5.96	119.98	117.00
1	AA	729	A	C4-C5-C6	5.96	119.98	117.00
1	AA	781	A	N3-C4-N9	5.96	132.16	127.40
1	AA	1508	A	N3-C4-N9	5.96	132.17	127.40
26	BA	71	A	N3-C4-N9	5.96	132.16	127.40
26	BA	181	A	C4-C5-C6	5.96	119.98	117.00
26	BA	430	A	N3-C4-N9	5.96	132.16	127.40
26	BA	721	A	C4-C5-C6	5.96	119.98	117.00
26	BA	1009	A	C4-C5-C6	5.96	119.98	117.00
26	BA	1070	A	N3-C4-N9	5.96	132.17	127.40
26	BA	1626	A	C4-C5-C6	5.96	119.98	117.00
26	BA	1650	A	C4-C5-C6	5.96	119.98	117.00
26	BA	2434	A	C4-C5-C6	5.96	119.98	117.00
26	BA	2757	A	N3-C4-N9	5.96	132.16	127.40
1	AA	321	A	C4-C5-C6	5.96	119.98	117.00
1	AA	465	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1146	A	N3-C4-N9	5.96	132.16	127.40
26	BA	71	A	C4-C5-C6	5.96	119.98	117.00
26	BA	793	A	C4-C5-C6	5.96	119.98	117.00
26	BA	1637	A	N3-C4-N9	5.96	132.16	127.40
1	AA	383	A	C4-C5-C6	5.95	119.98	117.00
1	AA	553	A	N3-C4-N9	5.95	132.16	127.40
1	AA	964	A	C4-C5-C6	5.95	119.98	117.00
1	AA	1340	A	N3-C4-N9	5.95	132.16	127.40
25	AY	35	A	C4-C5-C6	5.95	119.98	117.00
26	BA	144	A	C4-C5-C6	5.95	119.98	117.00
26	BA	204	A	C8-N9-C4	5.95	108.18	105.80
26	BA	505	A	N3-C4-N9	5.95	132.16	127.40
26	BA	1090	A	C4-C5-C6	5.95	119.98	117.00
26	BA	1789	A	C4-C5-C6	5.95	119.98	117.00
26	BA	262	A	C4-C5-C6	5.95	119.98	117.00
26	BA	2119	A	C4-C5-C6	5.95	119.98	117.00
26	BA	2468	A	N3-C4-N9	5.95	132.16	127.40
26	BA	2482	A	C4-C5-C6	5.95	119.98	117.00
1	AA	223	A	C4-C5-C6	5.95	119.97	117.00
1	AA	313	A	C4-C5-C6	5.95	119.97	117.00
1	AA	461	A	C4-C5-C6	5.95	119.97	117.00
1	AA	535	A	C4-C5-C6	5.95	119.97	117.00
1	AA	655	A	C4-C5-C6	5.95	119.98	117.00
1	AA	1004	A	N3-C4-N9	5.95	132.16	127.40
1	AA	1176	A	N3-C4-N9	5.95	132.16	127.40
26	BA	49	A	N3-C4-N9	5.95	132.16	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	104	A	C4-C5-C6	5.95	119.97	117.00
26	BA	197	A	C4-C5-C6	5.95	119.97	117.00
26	BA	1614	A	C4-C5-C6	5.95	119.97	117.00
27	BB	101	A	C4-C5-C6	5.95	119.97	117.00
1	AA	1227	A	C4-C5-C6	5.95	119.97	117.00
26	BA	342	A	C4-C5-C6	5.95	119.97	117.00
26	BA	502	A	C4-C5-C6	5.95	119.97	117.00
26	BA	925	A	N3-C4-N9	5.95	132.16	127.40
26	BA	1000	A	C4-C5-C6	5.95	119.97	117.00
26	BA	1020	A	C4-C5-C6	5.95	119.97	117.00
26	BA	1321	A	N3-C4-N9	5.95	132.16	127.40
26	BA	1579	A	N3-C4-N9	5.95	132.16	127.40
26	BA	2288	A	C4-C5-C6	5.95	119.97	117.00
26	BA	2369	A	C4-C5-C6	5.95	119.97	117.00
26	BA	2541	A	N3-C4-N9	5.95	132.16	127.40
26	BA	2738	A	C4-C5-C6	5.95	119.97	117.00
26	BA	2887	A	C4-C5-C6	5.95	119.97	117.00
27	BB	99	A	N3-C4-N9	5.95	132.16	127.40
1	AA	364	A	C4-C5-C6	5.95	119.97	117.00
26	BA	478	A	C4-C5-C6	5.95	119.97	117.00
1	AA	174	A	N3-C4-N9	5.95	132.16	127.40
1	AA	704	A	N3-C4-N9	5.95	132.16	127.40
1	AA	712	A	N3-C4-N9	5.95	132.16	127.40
1	AA	1274	A	C4-C5-C6	5.95	119.97	117.00
1	AA	1394	A	C8-N9-C4	5.95	108.18	105.80
26	BA	899	A	C4-C5-C6	5.95	119.97	117.00
26	BA	1672	A	C4-C5-C6	5.95	119.97	117.00
26	BA	1919	A	C4-C5-C6	5.95	119.97	117.00
26	BA	2476	A	C4-C5-C6	5.95	119.97	117.00
26	BA	2792	A	N3-C4-N9	5.95	132.16	127.40
24	AX	26	A	C4-C5-C6	5.94	119.97	117.00
24	AX	41	A	C4-C5-C6	5.94	119.97	117.00
26	BA	443	A	N3-C4-N9	5.94	132.16	127.40
26	BA	1069	A	C4-C5-C6	5.94	119.97	117.00
26	BA	1269	A	N3-C4-N9	5.94	132.16	127.40
26	BA	1302	A	C4-C5-C6	5.94	119.97	117.00
1	AA	964	A	N3-C4-N9	5.94	132.15	127.40
1	AA	1408	A	C8-N9-C4	5.94	108.18	105.80
1	AA	1531	A	N3-C4-N9	5.94	132.15	127.40
23	AW	14	A	C4-C5-C6	5.94	119.97	117.00
26	BA	1230	A	C4-C5-C6	5.94	119.97	117.00
26	BA	1569	A	C4-C5-C6	5.94	119.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1610	A	C4-C5-C6	5.94	119.97	117.00
26	BA	2126	A	C4-C5-C6	5.94	119.97	117.00
1	AA	65	A	C4-C5-C6	5.94	119.97	117.00
1	AA	109	A	N3-C4-N9	5.94	132.15	127.40
1	AA	250	A	C4-C5-C6	5.94	119.97	117.00
1	AA	482	A	C4-C5-C6	5.94	119.97	117.00
1	AA	595	A	N3-C4-N9	5.94	132.15	127.40
1	AA	675	A	N3-C4-N9	5.94	132.15	127.40
1	AA	718	A	C4-C5-C6	5.94	119.97	117.00
23	AW	73	A	N3-C4-N9	5.94	132.15	127.40
26	BA	19	A	C4-C5-C6	5.94	119.97	117.00
26	BA	91	A	C4-C5-C6	5.94	119.97	117.00
26	BA	482	A	N3-C4-N9	5.94	132.15	127.40
26	BA	878	A	C4-C5-C6	5.94	119.97	117.00
26	BA	1328	A	N3-C4-N9	5.94	132.15	127.40
26	BA	1754	A	C4-C5-C6	5.94	119.97	117.00
1	AA	554	A	N9-C4-C5	5.94	108.18	105.80
26	BA	541	A	N3-C4-N9	5.94	132.15	127.40
26	BA	2602	A	N3-C4-N9	5.94	132.15	127.40
1	AA	371	A	N3-C4-N9	5.94	132.15	127.40
1	AA	532	A	N3-C4-N9	5.94	132.15	127.40
26	BA	322	A	C4-C5-C6	5.94	119.97	117.00
26	BA	479	A	N3-C4-N9	5.94	132.15	127.40
26	BA	979	A	N3-C4-N9	5.94	132.15	127.40
26	BA	1096	A	C4-C5-C6	5.94	119.97	117.00
26	BA	1580	A	C4-C5-C6	5.94	119.97	117.00
26	BA	2117	A	N3-C4-N9	5.94	132.15	127.40
26	BA	2899	A	C4-C5-C6	5.94	119.97	117.00
27	BB	94	A	C4-C5-C6	5.94	119.97	117.00
1	AA	435	A	C4-C5-C6	5.94	119.97	117.00
1	AA	663	A	C4-C5-C6	5.94	119.97	117.00
1	AA	1216	A	C4-C5-C6	5.94	119.97	117.00
26	BA	227	A	C8-N9-C4	5.94	108.17	105.80
26	BA	412	A	C4-C5-C6	5.94	119.97	117.00
26	BA	1008	A	C4-C5-C6	5.94	119.97	117.00
26	BA	1284	A	C4-C5-C6	5.94	119.97	117.00
26	BA	1413	A	C4-C5-C6	5.94	119.97	117.00
26	BA	2070	A	C4-C5-C6	5.94	119.97	117.00
26	BA	2142	A	N3-C4-N9	5.94	132.15	127.40
26	BA	2270	A	C4-C5-C6	5.94	119.97	117.00
26	BA	2377	A	C4-C5-C6	5.94	119.97	117.00
1	AA	432	A	N3-C4-N9	5.93	132.15	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	532	A	C4-C5-C6	5.93	119.97	117.00
1	AA	959	A	C4-C5-C6	5.93	119.97	117.00
1	AA	1191	A	N3-C4-N9	5.93	132.15	127.40
26	BA	218	A	N3-C4-N9	5.93	132.15	127.40
26	BA	781	A	C4-C5-C6	5.93	119.97	117.00
26	BA	979	A	C4-C5-C6	5.93	119.97	117.00
26	BA	1008	A	N3-C4-N9	5.93	132.15	127.40
26	BA	1010	A	C4-C5-C6	5.93	119.97	117.00
26	BA	1028	A	C4-C5-C6	5.93	119.97	117.00
26	BA	1802	A	C4-C5-C6	5.93	119.97	117.00
26	BA	1936	A	N3-C4-N9	5.93	132.15	127.40
26	BA	2776	A	C8-N9-C4	5.93	108.17	105.80
1	AA	119	A	N3-C4-N9	5.93	132.15	127.40
1	AA	559	A	C4-C5-C6	5.93	119.97	117.00
1	AA	665	A	N9-C4-C5	5.93	108.17	105.80
1	AA	1201	A	C4-C5-C6	5.93	119.97	117.00
1	AA	1430	A	N3-C4-N9	5.93	132.15	127.40
26	BA	213	A	C4-C5-C6	5.93	119.97	117.00
26	BA	368	A	C4-C5-C6	5.93	119.97	117.00
26	BA	402	A	N3-C4-N9	5.93	132.15	127.40
26	BA	631	A	N3-C4-N9	5.93	132.15	127.40
26	BA	1126	A	C4-C5-C6	5.93	119.97	117.00
26	BA	1434	A	N3-C4-N9	5.93	132.15	127.40
26	BA	1503	A	C4-C5-C6	5.93	119.97	117.00
26	BA	1572	A	N3-C4-N9	5.93	132.15	127.40
26	BA	1853	A	C4-C5-C6	5.93	119.97	117.00
26	BA	2101	A	C4-C5-C6	5.93	119.97	117.00
26	BA	2274	A	C4-C5-C6	5.93	119.97	117.00
26	BA	2278	A	C4-C5-C6	5.93	119.97	117.00
26	BA	2284	A	C4-C5-C6	5.93	119.97	117.00
26	BA	2284	A	N3-C4-N9	5.93	132.15	127.40
26	BA	2753	A	C4-C5-C6	5.93	119.97	117.00
26	BA	2821	A	C4-C5-C6	5.93	119.97	117.00
27	BB	119	A	C4-C5-C6	5.93	119.97	117.00
1	AA	7	A	C4-C5-C6	5.93	119.97	117.00
1	AA	635	A	C4-C5-C6	5.93	119.97	117.00
1	AA	802	A	C4-C5-C6	5.93	119.97	117.00
1	AA	807	A	C4-C5-C6	5.93	119.97	117.00
1	AA	919	A	C4-C5-C6	5.93	119.97	117.00
26	BA	118	A	C4-C5-C6	5.93	119.97	117.00
26	BA	309	A	C4-C5-C6	5.93	119.97	117.00
26	BA	643	A	C4-C5-C6	5.93	119.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	661	A	C4-C5-C6	5.93	119.97	117.00
26	BA	981	A	C4-C5-C6	5.93	119.97	117.00
26	BA	1067	A	C4-C5-C6	5.93	119.97	117.00
26	BA	1321	A	C4-C5-C6	5.93	119.97	117.00
26	BA	2670	A	C4-C5-C6	5.93	119.97	117.00
26	BA	2750	A	C4-C5-C6	5.93	119.97	117.00
26	BA	2781	A	C4-C5-C6	5.93	119.97	117.00
27	BB	50	A	C4-C5-C6	5.93	119.97	117.00
1	AA	279	A	C4-C5-C6	5.93	119.97	117.00
1	AA	1375	A	C4-C5-C6	5.93	119.97	117.00
1	AA	1513	A	C4-C5-C6	5.93	119.97	117.00
26	BA	195	A	N3-C4-N9	5.93	132.14	127.40
26	BA	216	A	C4-C5-C6	5.93	119.96	117.00
26	BA	1098	A	C4-C5-C6	5.93	119.96	117.00
1	AA	228	A	N3-C4-N9	5.93	132.14	127.40
1	AA	274	A	C4-C5-C6	5.93	119.96	117.00
1	AA	1368	A	C8-N9-C4	5.93	108.17	105.80
1	AA	1441	A	C4-C5-C6	5.93	119.96	117.00
26	BA	631	A	C4-C5-C6	5.93	119.96	117.00
26	BA	632	A	N3-C4-N9	5.93	132.14	127.40
26	BA	792	A	N3-C4-N9	5.93	132.14	127.40
26	BA	2212	A	N3-C4-N9	5.93	132.14	127.40
26	BA	2893	A	N3-C4-N9	5.93	132.14	127.40
27	BB	50	A	N3-C4-N9	5.93	132.14	127.40
1	AA	139	A	C4-C5-C6	5.93	119.96	117.00
1	AA	460	A	N3-C4-N9	5.93	132.14	127.40
25	AY	9	A	N3-C4-N9	5.93	132.14	127.40
26	BA	91	A	N3-C4-N9	5.93	132.14	127.40
26	BA	616	A	N3-C4-N9	5.93	132.14	127.40
26	BA	1900	A	N3-C4-N9	5.93	132.14	127.40
26	BA	2530	A	C4-C5-C6	5.93	119.96	117.00
26	BA	2809	A	N3-C4-N9	5.93	132.14	127.40
27	BB	39	A	C4-C5-C6	5.93	119.96	117.00
27	BB	39	A	N3-C4-N9	5.93	132.14	127.40
26	BA	146	A	C4-C5-C6	5.92	119.96	117.00
26	BA	282	A	N3-C4-N9	5.92	132.14	127.40
26	BA	344	A	C4-C5-C6	5.92	119.96	117.00
26	BA	990	A	C8-N9-C4	5.92	108.17	105.80
26	BA	1544	A	C4-C5-C6	5.92	119.96	117.00
26	BA	1754	A	N3-C4-N9	5.92	132.14	127.40
26	BA	2388	A	C8-N9-C4	5.92	108.17	105.80
26	BA	2411	A	C4-C5-C6	5.92	119.96	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2425	A	C4-C5-C6	5.92	119.96	117.00
26	BA	2660	A	C4-C5-C6	5.92	119.96	117.00
27	BB	45	A	N3-C4-N9	5.92	132.14	127.40
1	AA	1219	A	N3-C4-N9	5.92	132.14	127.40
25	AY	66	A	C4-C5-C6	5.92	119.96	117.00
26	BA	146	A	N3-C4-N9	5.92	132.14	127.40
1	AA	441	A	C4-C5-C6	5.92	119.96	117.00
1	AA	649	A	C4-C5-C6	5.92	119.96	117.00
1	AA	768	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1042	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1105	A	C4-C5-C6	5.92	119.96	117.00
24	AX	58	A	C4-C5-C6	5.92	119.96	117.00
26	BA	28	A	N3-C4-N9	5.92	132.14	127.40
26	BA	222	A	N3-C4-N9	5.92	132.14	127.40
26	BA	492	A	N3-C4-N9	5.92	132.14	127.40
26	BA	715	A	N3-C4-N9	5.92	132.14	127.40
26	BA	1054	A	C4-C5-C6	5.92	119.96	117.00
26	BA	1858	A	N3-C4-N9	5.92	132.14	127.40
26	BA	1885	A	N3-C4-N9	5.92	132.14	127.40
26	BA	2700	A	N3-C4-N9	5.92	132.14	127.40
26	BA	2882	A	C4-C5-C6	5.92	119.96	117.00
1	AA	167	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1319	A	N3-C4-N9	5.92	132.14	127.40
1	AA	1375	A	N3-C4-N9	5.92	132.14	127.40
1	AA	1500	A	C4-C5-C6	5.92	119.96	117.00
26	BA	793	A	N3-C4-N9	5.92	132.14	127.40
26	BA	802	A	N3-C4-N9	5.92	132.14	127.40
26	BA	910	A	C4-C5-C6	5.92	119.96	117.00
1	AA	167	A	N3-C4-N9	5.92	132.13	127.40
1	AA	363	A	N3-C4-N9	5.92	132.13	127.40
1	AA	374	A	C4-C5-C6	5.92	119.96	117.00
1	AA	860	A	N3-C4-N9	5.92	132.13	127.40
1	AA	937	A	C4-C5-C6	5.92	119.96	117.00
26	BA	428	A	N3-C4-N9	5.92	132.13	127.40
26	BA	666	A	C4-C5-C6	5.92	119.96	117.00
26	BA	751	A	N3-C4-N9	5.92	132.13	127.40
26	BA	849	A	C4-C5-C6	5.92	119.96	117.00
26	BA	1151	A	N3-C4-N9	5.92	132.13	127.40
26	BA	1155	A	N9-C4-C5	5.92	108.17	105.80
26	BA	1384	A	C4-C5-C6	5.92	119.96	117.00
26	BA	1746	A	N3-C4-N9	5.92	132.13	127.40
26	BA	2227	A	C4-C5-C6	5.92	119.96	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2564	A	C4-C5-C6	5.92	119.96	117.00
26	BA	2893	A	C4-C5-C6	5.92	119.96	117.00
1	AA	77	A	C4-C5-C6	5.92	119.96	117.00
1	AA	414	A	N3-C4-N9	5.92	132.13	127.40
1	AA	1169	A	N3-C4-N9	5.92	132.13	127.40
1	AA	1288	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1434	A	C4-C5-C6	5.92	119.96	117.00
26	BA	94	A	N3-C4-N9	5.92	132.13	127.40
26	BA	626	A	C4-C5-C6	5.92	119.96	117.00
26	BA	943	A	N3-C4-N9	5.92	132.13	127.40
26	BA	1194	A	C4-C5-C6	5.92	119.96	117.00
26	BA	1393	A	C4-C5-C6	5.92	119.96	117.00
26	BA	1431	A	C4-C5-C6	5.92	119.96	117.00
26	BA	1586	A	C4-C5-C6	5.92	119.96	117.00
26	BA	2333	A	C8-N9-C4	5.92	108.17	105.80
1	AA	161	A	C4-C5-C6	5.92	119.96	117.00
25	AY	14	A	C4-C5-C6	5.92	119.96	117.00
26	BA	1046	A	C4-C5-C6	5.92	119.96	117.00
26	BA	2749	A	C4-C5-C6	5.92	119.96	117.00
27	BB	58	A	C4-C5-C6	5.92	119.96	117.00
1	AA	16	A	C8-N9-C4	5.91	108.17	105.80
1	AA	382	A	C4-C5-C6	5.91	119.96	117.00
1	AA	451	A	C4-C5-C6	5.91	119.96	117.00
1	AA	831	A	N3-C4-N9	5.91	132.13	127.40
1	AA	1299	A	C4-C5-C6	5.91	119.96	117.00
26	BA	272	A	C4-C5-C6	5.91	119.96	117.00
26	BA	412	A	N3-C4-N9	5.91	132.13	127.40
26	BA	522	A	N3-C4-N9	5.91	132.13	127.40
26	BA	1640	A	C4-C5-C6	5.91	119.96	117.00
26	BA	1801	A	C4-C5-C6	5.91	119.96	117.00
26	BA	1885	A	C4-C5-C6	5.91	119.96	117.00
1	AA	787	A	N3-C4-N9	5.91	132.13	127.40
1	AA	1236	A	N3-C4-N9	5.91	132.13	127.40
26	BA	332	A	N3-C4-N9	5.91	132.13	127.40
26	BA	1746	A	C4-C5-C6	5.91	119.96	117.00
26	BA	2205	A	N3-C4-N9	5.91	132.13	127.40
1	AA	16	A	C4-C5-C6	5.91	119.95	117.00
1	AA	949	A	N3-C4-N9	5.91	132.13	127.40
1	AA	1155	A	C4-C5-C6	5.91	119.96	117.00
1	AA	1287	A	C4-C5-C6	5.91	119.95	117.00
1	AA	1502	A	N3-C4-N9	5.91	132.13	127.40
26	BA	227	A	C4-C5-C6	5.91	119.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	504	A	N3-C4-N9	5.91	132.13	127.40
26	BA	556	A	N3-C4-N9	5.91	132.13	127.40
26	BA	1028	A	N3-C4-N9	5.91	132.13	127.40
26	BA	1392	A	N3-C4-N9	5.91	132.13	127.40
26	BA	1672	A	N3-C4-N9	5.91	132.13	127.40
26	BA	1801	A	N3-C4-N9	5.91	132.13	127.40
26	BA	2033	A	N9-C4-C5	5.91	108.17	105.80
26	BA	2340	A	C4-C5-C6	5.91	119.96	117.00
26	BA	2634	A	N3-C4-N9	5.91	132.13	127.40
1	AA	320	A	C4-C5-C6	5.91	119.95	117.00
1	AA	523	A	N3-C4-N9	5.91	132.13	127.40
1	AA	560	A	C4-C5-C6	5.91	119.95	117.00
1	AA	1171	A	N3-C4-N9	5.91	132.13	127.40
1	AA	1225	A	N3-C4-N9	5.91	132.13	127.40
1	AA	1306	A	N3-C4-N9	5.91	132.13	127.40
26	BA	352	A	C4-C5-C6	5.91	119.95	117.00
26	BA	878	A	N3-C4-N9	5.91	132.13	127.40
26	BA	1205	A	C4-C5-C6	5.91	119.95	117.00
1	AA	161	A	N3-C4-N9	5.91	132.13	127.40
1	AA	1329	A	N9-C4-C5	5.91	108.16	105.80
23	AW	69	A	C4-C5-C6	5.91	119.95	117.00
26	BA	222	A	C4-C5-C6	5.91	119.95	117.00
26	BA	423	A	N3-C4-N9	5.91	132.13	127.40
26	BA	2003	A	C4-C5-C6	5.91	119.95	117.00
26	BA	2478	A	C8-N9-C4	5.91	108.16	105.80
1	AA	81	A	N3-C4-N9	5.91	132.12	127.40
1	AA	784	A	N3-C4-N9	5.91	132.12	127.40
1	AA	969	A	C4-C5-C6	5.91	119.95	117.00
1	AA	1111	A	C4-C5-C6	5.91	119.95	117.00
25	AY	35	A	N3-C4-N9	5.91	132.12	127.40
26	BA	144	A	N3-C4-N9	5.91	132.12	127.40
26	BA	226	A	C4-C5-C6	5.91	119.95	117.00
26	BA	342	A	N3-C4-N9	5.91	132.12	127.40
26	BA	345	A	N3-C4-N9	5.91	132.12	127.40
26	BA	505	A	C8-N9-C4	5.91	108.16	105.80
26	BA	753	A	N3-C4-N9	5.91	132.12	127.40
26	BA	972	A	N3-C4-N9	5.91	132.12	127.40
26	BA	1156	A	C4-C5-C6	5.91	119.95	117.00
26	BA	1264	A	N3-C4-N9	5.91	132.12	127.40
26	BA	1354	A	N3-C4-N9	5.91	132.12	127.40
26	BA	1717	A	N3-C4-N9	5.91	132.12	127.40
26	BA	1757	A	C4-C5-C6	5.91	119.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1805	A	C4-C5-C6	5.91	119.95	117.00
26	BA	1847	A	N3-C4-N9	5.91	132.12	127.40
26	BA	1871	A	C4-C5-C6	5.91	119.95	117.00
26	BA	2820	A	C4-C5-C6	5.91	119.95	117.00
1	AA	101	A	C4-C5-C6	5.90	119.95	117.00
1	AA	695	A	N3-C4-N9	5.90	132.12	127.40
1	AA	715	A	C4-C5-C6	5.90	119.95	117.00
1	AA	767	A	C8-N9-C4	5.90	108.16	105.80
26	BA	861	A	C4-C5-C6	5.90	119.95	117.00
26	BA	1230	A	N3-C4-N9	5.90	132.12	127.40
26	BA	1322	A	C4-C5-C6	5.90	119.95	117.00
26	BA	1890	A	C4-C5-C6	5.90	119.95	117.00
26	BA	2886	A	N3-C4-N9	5.90	132.12	127.40
27	BB	115	A	N3-C4-N9	5.90	132.12	127.40
1	AA	8	A	N3-C4-N9	5.90	132.12	127.40
1	AA	199	A	C4-C5-C6	5.90	119.95	117.00
1	AA	780	A	N3-C4-N9	5.90	132.12	127.40
1	AA	1035	A	N3-C4-N9	5.90	132.12	127.40
1	AA	1151	A	C8-N9-C4	5.90	108.16	105.80
1	AA	1456	A	C4-C5-C6	5.90	119.95	117.00
25	AY	41	A	C4-C5-C6	5.90	119.95	117.00
26	BA	332	A	C8-N9-C4	5.90	108.16	105.80
26	BA	910	A	N3-C4-N9	5.90	132.12	127.40
26	BA	941	A	N3-C4-N9	5.90	132.12	127.40
26	BA	1054	A	N3-C4-N9	5.90	132.12	127.40
26	BA	1532	A	N3-C4-N9	5.90	132.12	127.40
26	BA	1938	A	N3-C4-N9	5.90	132.12	127.40
26	BA	2453	A	C4-C5-C6	5.90	119.95	117.00
26	BA	2635	A	N3-C4-N9	5.90	132.12	127.40
1	AA	130	A	N3-C4-N9	5.90	132.12	127.40
1	AA	189	A	N3-C4-N9	5.90	132.12	127.40
1	AA	716	A	N3-C4-N9	5.90	132.12	127.40
1	AA	1196	A	C4-C5-C6	5.90	119.95	117.00
1	AA	1456	A	N3-C4-N9	5.90	132.12	127.40
26	BA	14	A	N3-C4-N9	5.90	132.12	127.40
26	BA	348	A	N3-C4-N9	5.90	132.12	127.40
26	BA	453	A	N3-C4-N9	5.90	132.12	127.40
26	BA	1050	A	N3-C4-N9	5.90	132.12	127.40
26	BA	1262	A	C4-C5-C6	5.90	119.95	117.00
26	BA	1678	A	C4-C5-C6	5.90	119.95	117.00
26	BA	1717	A	C4-C5-C6	5.90	119.95	117.00
26	BA	2009	A	C8-N9-C4	5.90	108.16	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2682	A	C4-C5-C6	5.90	119.95	117.00
1	AA	1197	A	C4-C5-C6	5.90	119.95	117.00
26	BA	272	A	N3-C4-N9	5.90	132.12	127.40
26	BA	693	A	N3-C4-N9	5.90	132.12	127.40
1	AA	596	A	N3-C4-N9	5.90	132.12	127.40
1	AA	629	A	N3-C4-N9	5.90	132.12	127.40
1	AA	1055	A	C4-C5-C6	5.90	119.95	117.00
1	AA	1110	A	C4-C5-C6	5.90	119.95	117.00
1	AA	1447	A	C4-C5-C6	5.90	119.95	117.00
25	AY	21	A	N3-C4-N9	5.90	132.12	127.40
26	BA	203	A	N3-C4-N9	5.90	132.12	127.40
26	BA	439	A	N3-C4-N9	5.90	132.12	127.40
26	BA	592	A	C4-C5-C6	5.90	119.95	117.00
26	BA	613	A	N3-C4-N9	5.90	132.12	127.40
26	BA	1819	A	C4-C5-C6	5.90	119.95	117.00
26	BA	1977	A	N3-C4-N9	5.90	132.12	127.40
26	BA	2721	A	N3-C4-N9	5.90	132.12	127.40
1	AA	366	A	C4-C5-C6	5.90	119.95	117.00
1	AA	900	A	N3-C4-N9	5.90	132.12	127.40
1	AA	1082	A	C4-C5-C6	5.90	119.95	117.00
1	AA	1433	A	N3-C4-N9	5.90	132.12	127.40
26	BA	84	A	C8-N9-C4	5.90	108.16	105.80
26	BA	172	A	C4-C5-C6	5.90	119.95	117.00
26	BA	614	A	C4-C5-C6	5.90	119.95	117.00
26	BA	752	A	N3-C4-N9	5.90	132.12	127.40
26	BA	1304	A	C4-C5-C6	5.90	119.95	117.00
26	BA	1528	A	N3-C4-N9	5.90	132.12	127.40
26	BA	1722	A	N3-C4-N9	5.90	132.12	127.40
1	AA	160	A	C4-C5-C6	5.89	119.95	117.00
1	AA	382	A	N3-C4-N9	5.89	132.12	127.40
1	AA	520	A	C4-C5-C6	5.89	119.95	117.00
1	AA	1016	A	C4-C5-C6	5.89	119.95	117.00
1	AA	1254	A	N3-C4-N9	5.89	132.12	127.40
1	AA	1428	A	C4-C5-C6	5.89	119.95	117.00
1	AA	1534	A	C4-C5-C6	5.89	119.95	117.00
26	BA	454	A	C4-C5-N7	-5.89	107.75	110.70
26	BA	590	A	C4-C5-C6	5.89	119.95	117.00
26	BA	782	A	C4-C5-C6	5.89	119.95	117.00
26	BA	866	A	N3-C4-N9	5.89	132.12	127.40
26	BA	1373	A	N3-C4-N9	5.89	132.12	127.40
26	BA	1759	A	C4-C5-C6	5.89	119.95	117.00
26	BA	2377	A	N3-C4-N9	5.89	132.12	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2425	A	N3-C4-N9	5.89	132.12	127.40
26	BA	2439	A	C8-N9-C4	5.89	108.16	105.80
1	AA	288	A	C4-C5-C6	5.89	119.95	117.00
1	AA	509	A	N3-C4-N9	5.89	132.11	127.40
1	AA	1169	A	C4-C5-C6	5.89	119.95	117.00
23	AW	21	A	C4-C5-C6	5.89	119.95	117.00
26	BA	63	A	N3-C4-N9	5.89	132.11	127.40
26	BA	182	A	N3-C4-N9	5.89	132.11	127.40
26	BA	586	A	C4-C5-C6	5.89	119.95	117.00
26	BA	699	A	C4-C5-C6	5.89	119.95	117.00
26	BA	975	A	N3-C4-N9	5.89	132.11	127.40
26	BA	1552	A	C4-C5-C6	5.89	119.95	117.00
26	BA	1821	A	C4-C5-C6	5.89	119.95	117.00
26	BA	1900	A	C8-N9-C4	5.89	108.16	105.80
26	BA	2037	A	C8-N9-C4	5.89	108.16	105.80
26	BA	2369	A	N3-C4-N9	5.89	132.12	127.40
1	AA	747	A	C4-C5-C6	5.89	119.94	117.00
26	BA	95	A	C4-C5-C6	5.89	119.95	117.00
26	BA	718	A	N3-C4-N9	5.89	132.11	127.40
26	BA	947	A	C8-N9-C4	5.89	108.16	105.80
26	BA	1609	A	C4-C5-C6	5.89	119.95	117.00
1	AA	171	A	N9-C4-C5	5.89	108.16	105.80
1	AA	694	A	N3-C4-N9	5.89	132.11	127.40
1	AA	792	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1254	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1280	A	N3-C4-N9	5.89	132.11	127.40
1	AA	1285	A	C4-C5-C6	5.89	119.94	117.00
23	AW	66	A	C4-C5-C6	5.89	119.94	117.00
26	BA	1597	A	C4-C5-C6	5.89	119.94	117.00
26	BA	2158	A	C4-C5-C6	5.89	119.94	117.00
26	BA	2705	A	N3-C4-N9	5.89	132.11	127.40
1	AA	642	A	N3-C4-N9	5.89	132.11	127.40
1	AA	946	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1067	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1346	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1349	A	N3-C4-N9	5.89	132.11	127.40
23	AW	41	A	C4-C5-C6	5.89	119.94	117.00
26	BA	44	A	N3-C4-N9	5.89	132.11	127.40
26	BA	643	A	N3-C4-N9	5.89	132.11	127.40
26	BA	1253	A	N3-C4-N9	5.89	132.11	127.40
26	BA	1665	A	C4-C5-C6	5.89	119.94	117.00
26	BA	1966	A	N3-C4-N9	5.89	132.11	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2733	A	N3-C4-N9	5.89	132.11	127.40
26	BA	2851	A	C4-C5-C6	5.89	119.94	117.00
26	BA	2873	A	N3-C4-N9	5.89	132.11	127.40
1	AA	3	A	C4-C5-C6	5.89	119.94	117.00
1	AA	303	A	N3-C4-N9	5.89	132.11	127.40
1	AA	559	A	N3-C4-N9	5.89	132.11	127.40
1	AA	1130	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1311	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1398	A	C4-C5-C6	5.89	119.94	117.00
26	BA	172	A	N3-C4-N9	5.89	132.11	127.40
26	BA	368	A	N3-C4-N9	5.89	132.11	127.40
26	BA	477	A	C4-C5-C6	5.89	119.94	117.00
26	BA	603	A	C4-C5-C6	5.89	119.94	117.00
26	BA	661	A	N3-C4-N9	5.89	132.11	127.40
26	BA	666	A	N3-C4-N9	5.89	132.11	127.40
26	BA	911	A	C4-C5-C6	5.89	119.94	117.00
26	BA	1477	A	N3-C4-N9	5.89	132.11	127.40
26	BA	1505	A	N3-C4-N9	5.89	132.11	127.40
26	BA	2411	A	N3-C4-N9	5.89	132.11	127.40
1	AA	181	A	N3-C4-N9	5.88	132.11	127.40
1	AA	325	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1092	A	C4-C5-C6	5.88	119.94	117.00
26	BA	1129	A	C4-C5-C6	5.88	119.94	117.00
26	BA	1302	A	N3-C4-N9	5.88	132.11	127.40
26	BA	1900	A	C4-C5-C6	5.88	119.94	117.00
26	BA	1937	A	N9-C4-C5	5.88	108.15	105.80
26	BA	1998	A	N3-C4-N9	5.88	132.11	127.40
26	BA	2042	A	N3-C4-N9	5.88	132.11	127.40
26	BA	2541	A	C4-C5-C6	5.88	119.94	117.00
26	BA	2600	A	C4-C5-C6	5.88	119.94	117.00
27	BB	46	A	C4-C5-C6	5.88	119.94	117.00
1	AA	673	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1394	A	N3-C4-N9	5.88	132.11	127.40
26	BA	705	A	C8-N9-C4	5.88	108.15	105.80
26	BA	716	A	N3-C4-N9	5.88	132.11	127.40
26	BA	782	A	N3-C4-N9	5.88	132.11	127.40
26	BA	1134	A	C4-C5-C6	5.88	119.94	117.00
26	BA	2426	A	C4-C5-C6	5.88	119.94	117.00
1	AA	28	A	N3-C4-N9	5.88	132.11	127.40
1	AA	696	A	N3-C4-N9	5.88	132.11	127.40
1	AA	1179	A	C4-C5-C6	5.88	119.94	117.00
26	BA	101	A	N3-C4-N9	5.88	132.10	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	722	A	N3-C4-N9	5.88	132.10	127.40
26	BA	1143	A	N3-C4-N9	5.88	132.10	127.40
26	BA	1773	A	N3-C4-N9	5.88	132.11	127.40
26	BA	1780	A	C4-C5-C6	5.88	119.94	117.00
26	BA	1938	A	C4-C5-C6	5.88	119.94	117.00
27	BB	66	A	N3-C4-N9	5.88	132.10	127.40
22	AV	21	A	C8-N9-C4	5.88	108.15	105.80
26	BA	181	A	N3-C4-N9	5.88	132.10	127.40
26	BA	1214	A	N3-C4-N9	5.88	132.10	127.40
26	BA	2090	A	C8-N9-C4	5.88	108.15	105.80
26	BA	2426	A	N3-C4-N9	5.88	132.10	127.40
26	BA	2435	A	C4-C5-C6	5.88	119.94	117.00
26	BA	2679	A	C4-C5-C6	5.88	119.94	117.00
27	BB	66	A	C4-C5-C6	5.88	119.94	117.00
1	AA	313	A	N3-C4-N9	5.88	132.10	127.40
1	AA	461	A	N3-C4-N9	5.88	132.10	127.40
1	AA	913	A	C8-N9-C4	5.88	108.15	105.80
1	AA	1446	A	N3-C4-N9	5.88	132.10	127.40
26	BA	742	A	C4-C5-C6	5.88	119.94	117.00
26	BA	1080	A	C4-C5-C6	5.88	119.94	117.00
26	BA	1698	A	N3-C4-N9	5.88	132.10	127.40
26	BA	1700	A	C4-C5-C6	5.88	119.94	117.00
26	BA	1783	A	N9-C4-C5	5.88	108.15	105.80
26	BA	1809	A	N3-C4-N9	5.88	132.10	127.40
26	BA	2660	A	N3-C4-N9	5.88	132.10	127.40
26	BA	2749	A	N3-C4-N9	5.88	132.10	127.40
1	AA	459	A	C4-C5-C6	5.88	119.94	117.00
1	AA	574	A	C4-C5-C6	5.88	119.94	117.00
1	AA	819	A	C4-C5-C6	5.88	119.94	117.00
1	AA	914	A	C4-C5-C6	5.88	119.94	117.00
24	AX	76	A	C4-C5-C6	5.88	119.94	117.00
25	AY	9	A	C4-C5-C6	5.88	119.94	117.00
26	BA	270	A	C4-C5-C6	5.88	119.94	117.00
26	BA	299	A	N3-C4-N9	5.88	132.10	127.40
26	BA	1937	A	C4-C5-N7	-5.88	107.76	110.70
26	BA	2199	A	C4-C5-C6	5.88	119.94	117.00
26	BA	2392	A	N3-C4-N9	5.88	132.10	127.40
26	BA	2497	A	N3-C4-N9	5.88	132.10	127.40
26	BA	2736	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1229	A	C4-C5-C6	5.88	119.94	117.00
26	BA	1952	A	N3-C4-N9	5.88	132.10	127.40
26	BA	2632	A	C4-C5-C6	5.88	119.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	65	A	N3-C4-N9	5.87	132.10	127.40
1	AA	197	A	C4-C5-C6	5.87	119.94	117.00
1	AA	547	A	C8-N9-C4	5.87	108.15	105.80
1	AA	630	A	N3-C4-N9	5.87	132.10	127.40
1	AA	1251	A	N3-C4-N9	5.87	132.10	127.40
1	AA	1503	A	N3-C4-N9	5.87	132.10	127.40
26	BA	44	A	C4-C5-C6	5.87	119.94	117.00
26	BA	1927	A	N3-C4-N9	5.87	132.10	127.40
26	BA	2757	A	C4-C5-C6	5.87	119.94	117.00
1	AA	1213	A	C4-C5-C6	5.87	119.94	117.00
26	BA	6	A	N3-C4-N9	5.87	132.10	127.40
26	BA	13	A	N3-C4-N9	5.87	132.10	127.40
26	BA	156	A	C4-C5-C6	5.87	119.94	117.00
26	BA	877	A	N3-C4-N9	5.87	132.10	127.40
26	BA	1111	A	N3-C4-N9	5.87	132.10	127.40
26	BA	1383	A	N3-C4-N9	5.87	132.10	127.40
26	BA	1785	A	N9-C4-C5	5.87	108.15	105.80
26	BA	2070	A	N9-C4-C5	5.87	108.15	105.80
26	BA	2097	A	N3-C4-N9	5.87	132.10	127.40
26	BA	2872	A	C4-C5-C6	5.87	119.94	117.00
1	AA	59	A	N3-C4-N9	5.87	132.10	127.40
1	AA	975	A	C4-C5-C6	5.87	119.94	117.00
1	AA	1046	A	C4-C5-C6	5.87	119.94	117.00
26	BA	896	A	C4-C5-C6	5.87	119.94	117.00
1	AA	325	A	N3-C4-N9	5.87	132.09	127.40
1	AA	1374	A	C8-N9-C4	5.87	108.15	105.80
26	BA	226	A	N3-C4-N9	5.87	132.09	127.40
26	BA	309	A	N3-C4-N9	5.87	132.09	127.40
26	BA	497	A	N3-C4-N9	5.87	132.09	127.40
26	BA	1027	A	N3-C4-N9	5.87	132.09	127.40
26	BA	1073	A	C4-C5-C6	5.87	119.93	117.00
26	BA	1246	A	C4-C5-C6	5.87	119.93	117.00
26	BA	1268	A	N3-C4-N9	5.87	132.09	127.40
26	BA	1336	A	C4-C5-C6	5.87	119.93	117.00
26	BA	1614	A	N3-C4-N9	5.87	132.10	127.40
26	BA	2572	A	C8-N9-C4	5.87	108.15	105.80
26	BA	2705	A	C4-C5-C6	5.87	119.93	117.00
26	BA	2850	A	N3-C4-N9	5.87	132.09	127.40
1	AA	2	A	C4-C5-C6	5.87	119.93	117.00
23	AW	58	A	N3-C4-N9	5.87	132.09	127.40
1	AA	78	A	C4-C5-C6	5.87	119.93	117.00
1	AA	143	A	C4-C5-C6	5.87	119.93	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	609	A	C4-C5-C6	5.87	119.93	117.00
1	AA	1377	A	N3-C4-N9	5.87	132.09	127.40
1	AA	1465	A	N3-C4-N9	5.87	132.09	127.40
25	AY	38	A	C8-N9-C4	5.87	108.15	105.80
25	AY	41	A	N3-C4-N9	5.87	132.09	127.40
26	BA	21	A	N3-C4-N9	5.87	132.09	127.40
26	BA	905	A	N9-C4-C5	5.87	108.15	105.80
26	BA	1431	A	N3-C4-N9	5.87	132.09	127.40
26	BA	1701	A	C4-C5-C6	5.87	119.93	117.00
1	AA	1000	A	C4-C5-C6	5.86	119.93	117.00
24	AX	26	A	N3-C4-N9	5.86	132.09	127.40
26	BA	219	A	N3-C4-N9	5.86	132.09	127.40
26	BA	503	A	N3-C4-N9	5.86	132.09	127.40
26	BA	927	A	C4-C5-C6	5.86	119.93	117.00
26	BA	1070	A	C4-C5-C6	5.86	119.93	117.00
26	BA	1272	A	N3-C4-N9	5.86	132.09	127.40
26	BA	1302	A	C8-N9-C4	5.86	108.15	105.80
26	BA	1366	A	C4-C5-C6	5.86	119.93	117.00
26	BA	1711	A	N3-C4-N9	5.86	132.09	127.40
26	BA	1808	A	C4-C5-C6	5.86	119.93	117.00
26	BA	2134	A	C4-C5-C6	5.86	119.93	117.00
26	BA	2227	A	N3-C4-N9	5.86	132.09	127.40
1	AA	344	A	N3-C4-N9	5.86	132.09	127.40
1	AA	572	A	C4-C5-C6	5.86	119.93	117.00
1	AA	845	A	N3-C4-N9	5.86	132.09	127.40
23	AW	21	A	N3-C4-N9	5.86	132.09	127.40
26	BA	2183	A	C4-C5-C6	5.86	119.93	117.00
1	AA	583	A	C4-C5-C6	5.86	119.93	117.00
1	AA	635	A	N3-C4-N9	5.86	132.09	127.40
1	AA	676	A	N3-C4-N9	5.86	132.09	127.40
1	AA	749	A	C4-C5-C6	5.86	119.93	117.00
1	AA	767	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1251	A	C4-C5-C6	5.86	119.93	117.00
25	AY	58	A	C4-C5-C6	5.86	119.93	117.00
26	BA	608	A	C4-C5-C6	5.86	119.93	117.00
26	BA	637	A	C4-C5-C6	5.86	119.93	117.00
26	BA	788	A	C4-C5-C6	5.86	119.93	117.00
26	BA	1032	A	C4-C5-C6	5.86	119.93	117.00
26	BA	1085	A	N3-C4-N9	5.86	132.09	127.40
26	BA	1366	A	N3-C4-N9	5.86	132.09	127.40
26	BA	1618	A	N3-C4-N9	5.86	132.09	127.40
26	BA	2268	A	N3-C4-N9	5.86	132.09	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2317	A	N3-C4-N9	5.86	132.09	127.40
27	BB	52	A	N3-C4-N9	5.86	132.09	127.40
1	AA	807	A	N3-C4-N9	5.86	132.09	127.40
1	AA	1408	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1480	A	C4-C5-C6	5.86	119.93	117.00
23	AW	38	A	N3-C4-N9	5.86	132.09	127.40
26	BA	1322	A	N3-C4-N9	5.86	132.09	127.40
26	BA	1596	A	C4-C5-C6	5.86	119.93	117.00
26	BA	2173	A	N3-C4-N9	5.86	132.09	127.40
1	AA	50	A	C4-C5-C6	5.86	119.93	117.00
1	AA	80	A	C4-C5-C6	5.86	119.93	117.00
1	AA	155	A	C4-C5-C6	5.86	119.93	117.00
1	AA	315	A	C4-C5-C6	5.86	119.93	117.00
1	AA	366	A	N3-C4-N9	5.86	132.09	127.40
1	AA	1036	A	N3-C4-N9	5.86	132.09	127.40
1	AA	1101	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1518	A	C4-C5-C6	5.86	119.93	117.00
22	AV	21	A	C4-C5-C6	5.86	119.93	117.00
22	AV	22	A	C4-C5-C6	5.86	119.93	117.00
26	BA	216	A	N3-C4-N9	5.86	132.09	127.40
26	BA	900	A	N3-C4-N9	5.86	132.09	127.40
26	BA	1127	A	N3-C4-N9	5.86	132.09	127.40
26	BA	1347	A	C4-C5-C6	5.86	119.93	117.00
26	BA	1650	A	N3-C4-N9	5.86	132.09	127.40
26	BA	2826	A	C4-C5-C6	5.86	119.93	117.00
27	BB	119	A	N3-C4-N9	5.86	132.09	127.40
1	AA	120	A	C4-C5-C6	5.86	119.93	117.00
1	AA	181	A	C4-C5-C6	5.86	119.93	117.00
1	AA	205	A	N3-C4-N9	5.86	132.08	127.40
1	AA	609	A	N3-C4-N9	5.86	132.08	127.40
1	AA	648	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1360	A	N3-C4-N9	5.86	132.09	127.40
23	AW	69	A	N3-C4-N9	5.86	132.08	127.40
24	AX	21	A	N3-C4-N9	5.86	132.09	127.40
24	AX	76	A	N3-C4-N9	5.86	132.08	127.40
26	BA	347	A	N3-C4-N9	5.86	132.08	127.40
26	BA	429	A	N3-C4-N9	5.86	132.08	127.40
26	BA	1096	A	N3-C4-N9	5.86	132.08	127.40
26	BA	1678	A	N3-C4-N9	5.86	132.09	127.40
26	BA	1762	A	N3-C4-N9	5.86	132.09	127.40
26	BA	2003	A	N3-C4-N9	5.86	132.08	127.40
26	BA	2378	A	N3-C4-N9	5.86	132.08	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BB	109	A	N3-C4-N9	5.86	132.08	127.40
1	AA	19	A	N3-C4-N9	5.85	132.08	127.40
1	AA	1252	A	N3-C4-N9	5.85	132.08	127.40
1	AA	1398	A	N3-C4-N9	5.85	132.08	127.40
25	AY	26	A	C4-C5-C6	5.85	119.93	117.00
26	BA	849	A	N3-C4-N9	5.85	132.08	127.40
26	BA	996	A	N3-C4-N9	5.85	132.08	127.40
26	BA	2433	A	N3-C4-N9	5.85	132.08	127.40
1	AA	8	A	C4-C5-C6	5.85	119.93	117.00
1	AA	120	A	N3-C4-N9	5.85	132.08	127.40
1	AA	160	A	N3-C4-N9	5.85	132.08	127.40
1	AA	766	A	N9-C4-C5	5.85	108.14	105.80
1	AA	937	A	N3-C4-N9	5.85	132.08	127.40
1	AA	1285	A	C8-N9-C4	5.85	108.14	105.80
26	BA	616	A	C8-N9-C4	5.85	108.14	105.80
26	BA	928	A	N3-C4-N9	5.85	132.08	127.40
26	BA	980	A	C4-C5-C6	5.85	119.93	117.00
26	BA	1014	A	N9-C4-C5	5.85	108.14	105.80
26	BA	1384	A	N3-C4-N9	5.85	132.08	127.40
26	BA	1420	A	C4-C5-C6	5.85	119.93	117.00
26	BA	1597	A	N3-C4-N9	5.85	132.08	127.40
26	BA	1616	A	C4-C5-C6	5.85	119.93	117.00
26	BA	1665	A	N3-C4-N9	5.85	132.08	127.40
26	BA	2030	A	C4-C5-C6	5.85	119.93	117.00
26	BA	2432	A	N3-C4-N9	5.85	132.08	127.40
26	BA	2572	A	C4-C5-C6	5.85	119.93	117.00
26	BA	2821	A	N3-C4-N9	5.85	132.08	127.40
26	BA	2851	A	N3-C4-N9	5.85	132.08	127.40
1	AA	1019	A	C4-C5-C6	5.85	119.92	117.00
22	AV	17	A	N3-C4-N9	5.85	132.08	127.40
26	BA	126	A	C4-C5-C6	5.85	119.92	117.00
26	BA	217	A	C4-C5-C6	5.85	119.93	117.00
26	BA	310	A	C8-N9-C4	5.85	108.14	105.80
26	BA	507	A	C4-C5-C6	5.85	119.93	117.00
26	BA	1336	A	N3-C4-N9	5.85	132.08	127.40
26	BA	1403	A	N3-C4-N9	5.85	132.08	127.40
1	AA	51	A	C8-N9-C4	5.85	108.14	105.80
1	AA	1082	A	N3-C4-N9	5.85	132.08	127.40
1	AA	1110	A	N3-C4-N9	5.85	132.08	127.40
1	AA	1163	A	N3-C4-N9	5.85	132.08	127.40
26	BA	91	A	C8-N9-C4	5.85	108.14	105.80
26	BA	497	A	C4-C5-C6	5.85	119.92	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	727	A	N3-C4-N9	5.85	132.08	127.40
26	BA	789	A	N3-C4-N9	5.85	132.08	127.40
26	BA	959	A	N3-C4-N9	5.85	132.08	127.40
26	BA	1427	A	C8-N9-C4	5.85	108.14	105.80
26	BA	1596	A	N3-C4-N9	5.85	132.08	127.40
26	BA	1701	A	N3-C4-N9	5.85	132.08	127.40
26	BA	2241	A	C4-C5-C6	5.85	119.92	117.00
26	BA	2281	A	C4-C5-C6	5.85	119.92	117.00
1	AA	250	A	N3-C4-N9	5.85	132.08	127.40
1	AA	1157	A	C8-N9-C4	5.85	108.14	105.80
1	AA	1204	A	C4-C5-C6	5.85	119.92	117.00
1	AA	1368	A	C4-C5-C6	5.85	119.92	117.00
1	AA	1500	A	N3-C4-N9	5.85	132.08	127.40
26	BA	432	A	N3-C4-N9	5.85	132.08	127.40
26	BA	616	A	C4-C5-C6	5.85	119.92	117.00
26	BA	833	A	N3-C4-N9	5.85	132.08	127.40
26	BA	1284	A	N3-C4-N9	5.85	132.08	127.40
26	BA	1307	A	N3-C4-N9	5.85	132.08	127.40
26	BA	1713	A	N3-C4-N9	5.85	132.08	127.40
26	BA	2005	A	N3-C4-N9	5.85	132.08	127.40
26	BA	2764	A	N9-C4-C5	5.85	108.14	105.80
1	AA	547	A	C4-C5-C6	5.85	119.92	117.00
1	AA	815	A	C4-C5-C6	5.85	119.92	117.00
1	AA	1431	A	N3-C4-N9	5.85	132.08	127.40
26	BA	501	A	N3-C4-N9	5.85	132.08	127.40
1	AA	131	A	C8-N9-C4	5.84	108.14	105.80
1	AA	336	A	C4-C5-C6	5.84	119.92	117.00
1	AA	687	A	C8-N9-C4	5.84	108.14	105.80
1	AA	889	A	C8-N9-C4	5.84	108.14	105.80
1	AA	1197	A	N3-C4-N9	5.84	132.07	127.40
1	AA	1434	A	N3-C4-N9	5.84	132.07	127.40
25	AY	58	A	N3-C4-N9	5.84	132.07	127.40
26	BA	592	A	N3-C4-N9	5.84	132.07	127.40
26	BA	602	A	N3-C4-N9	5.84	132.08	127.40
26	BA	670	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1095	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1098	A	N3-C4-N9	5.84	132.08	127.40
26	BA	1354	A	C8-N9-C4	5.84	108.14	105.80
26	BA	1953	A	C4-C5-C6	5.84	119.92	117.00
26	BA	2158	A	C8-N9-C4	5.84	108.14	105.80
1	AA	236	A	N3-C4-N9	5.84	132.07	127.40
1	AA	790	A	N3-C4-N9	5.84	132.07	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	221	A	N3-C4-N9	5.84	132.07	127.40
26	BA	472	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1754	A	C8-N9-C4	5.84	108.14	105.80
26	BA	2418	A	C4-C5-N7	-5.84	107.78	110.70
1	AA	353	A	C8-N9-C4	5.84	108.14	105.80
1	AA	560	A	N3-C4-N9	5.84	132.07	127.40
1	AA	906	A	N3-C4-N9	5.84	132.07	127.40
1	AA	1130	A	N3-C4-N9	5.84	132.07	127.40
1	AA	1201	A	C8-N9-C4	5.84	108.14	105.80
1	AA	1213	A	N3-C4-N9	5.84	132.07	127.40
25	AY	14	A	N3-C4-N9	5.84	132.07	127.40
26	BA	74	A	C8-N9-C4	5.84	108.14	105.80
26	BA	119	A	C8-N9-C4	5.84	108.14	105.80
26	BA	199	A	C4-C5-C6	5.84	119.92	117.00
26	BA	608	A	N3-C4-N9	5.84	132.07	127.40
26	BA	655	A	C8-N9-C4	5.84	108.14	105.80
26	BA	936	A	C4-C5-C6	5.84	119.92	117.00
26	BA	1156	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1175	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1253	A	C8-N9-C4	5.84	108.14	105.80
26	BA	1367	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1544	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1551	A	C4-C5-C6	5.84	119.92	117.00
26	BA	2117	A	C4-C5-C6	5.84	119.92	117.00
26	BA	2542	A	C4-C5-C6	5.84	119.92	117.00
26	BA	2654	A	N3-C4-N9	5.84	132.07	127.40
1	AA	320	A	N3-C4-N9	5.84	132.07	127.40
1	AA	498	A	C4-C5-C6	5.84	119.92	117.00
1	AA	600	A	N3-C4-N9	5.84	132.07	127.40
1	AA	622	A	N9-C4-C5	5.84	108.14	105.80
1	AA	1257	A	N3-C4-N9	5.84	132.07	127.40
26	BA	95	A	N3-C4-N9	5.84	132.07	127.40
26	BA	241	A	C8-N9-C4	5.84	108.14	105.80
26	BA	344	A	N3-C4-N9	5.84	132.07	127.40
26	BA	483	A	C4-C5-C6	5.84	119.92	117.00
26	BA	614	A	N3-C4-N9	5.84	132.07	127.40
26	BA	727	A	C8-N9-C4	5.84	108.14	105.80
26	BA	979	A	C8-N9-C4	5.84	108.14	105.80
26	BA	1308	A	C4-C5-N7	-5.84	107.78	110.70
26	BA	1580	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1632	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1757	A	C8-N9-C4	5.84	108.14	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1877	A	N3-C4-N9	5.84	132.07	127.40
26	BA	2060	A	N3-C4-N9	5.84	132.07	127.40
26	BA	2169	A	C4-C5-C6	5.84	119.92	117.00
26	BA	2198	A	C4-C5-C6	5.84	119.92	117.00
26	BA	2564	A	N3-C4-N9	5.84	132.07	127.40
1	AA	72	A	C4-C5-C6	5.84	119.92	117.00
1	AA	547	A	N3-C4-N9	5.84	132.07	127.40
1	AA	554	A	C4-C5-N7	-5.84	107.78	110.70
1	AA	1055	A	C8-N9-C4	5.84	108.14	105.80
26	BA	1205	A	N3-C4-N9	5.84	132.07	127.40
26	BA	2813	A	N3-C4-N9	5.84	132.07	127.40
1	AA	66	A	C4-C5-C6	5.84	119.92	117.00
1	AA	120	A	C8-N9-C4	5.84	108.14	105.80
1	AA	149	A	N3-C4-N9	5.84	132.07	127.40
1	AA	223	A	N3-C4-N9	5.84	132.07	127.40
1	AA	321	A	N3-C4-N9	5.84	132.07	127.40
1	AA	338	A	C4-C5-C6	5.84	119.92	117.00
1	AA	790	A	C4-C5-C6	5.84	119.92	117.00
1	AA	915	A	C8-N9-C4	5.84	108.14	105.80
1	AA	1274	A	N3-C4-N9	5.84	132.07	127.40
26	BA	783	A	N9-C4-C5	5.84	108.13	105.80
26	BA	980	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1134	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1593	A	C4-C5-C6	5.84	119.92	117.00
26	BA	1805	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1871	A	N3-C4-N9	5.84	132.07	127.40
26	BA	1889	A	N3-C4-N9	5.84	132.07	127.40
26	BA	2071	A	C8-N9-C4	5.84	108.14	105.80
26	BA	2170	A	N3-C4-N9	5.84	132.07	127.40
26	BA	2199	A	N3-C4-N9	5.84	132.07	127.40
26	BA	2274	A	N3-C4-N9	5.84	132.07	127.40
26	BA	2810	A	N3-C4-N9	5.84	132.07	127.40
1	AA	10	A	C4-C5-C6	5.83	119.92	117.00
1	AA	1180	A	N3-C4-N9	5.83	132.07	127.40
1	AA	1408	A	N3-C4-N9	5.83	132.07	127.40
26	BA	125	A	C4-C5-C6	5.83	119.92	117.00
26	BA	1495	A	N3-C4-N9	5.83	132.07	127.40
26	BA	2281	A	N3-C4-N9	5.83	132.07	127.40
1	AA	747	A	N3-C4-N9	5.83	132.07	127.40
1	AA	1188	A	N3-C4-N9	5.83	132.07	127.40
23	AW	31	A	N3-C4-N9	5.83	132.07	127.40
26	BA	920	A	N3-C4-N9	5.83	132.07	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1126	A	N3-C4-N9	5.83	132.07	127.40
26	BA	1591	A	C8-N9-C4	5.83	108.13	105.80
26	BA	2005	A	C4-C5-C6	5.83	119.92	117.00
26	BA	2070	A	C4-C5-N7	-5.83	107.78	110.70
26	BA	2346	A	N3-C4-N9	5.83	132.07	127.40
27	BB	94	A	N3-C4-N9	5.83	132.07	127.40
1	AA	51	A	N3-C4-N9	5.83	132.06	127.40
1	AA	819	A	N3-C4-N9	5.83	132.06	127.40
1	AA	1201	A	N3-C4-N9	5.83	132.06	127.40
1	AA	1429	A	C8-N9-C4	5.83	108.13	105.80
26	BA	735	A	N3-C4-N9	5.83	132.06	127.40
26	BA	1039	A	N3-C4-N9	5.83	132.06	127.40
26	BA	1677	A	C4-C5-C6	5.83	119.92	117.00
26	BA	2060	A	C8-N9-C4	5.83	108.13	105.80
27	BB	101	A	N3-C4-N9	5.83	132.07	127.40
1	AA	309	A	C4-C5-C6	5.83	119.92	117.00
1	AA	946	A	N3-C4-N9	5.83	132.06	127.40
26	BA	2883	A	C8-N9-C4	5.83	108.13	105.80
1	AA	72	A	N3-C4-N9	5.83	132.06	127.40
1	AA	262	A	N3-C4-N9	5.83	132.06	127.40
1	AA	279	A	N3-C4-N9	5.83	132.06	127.40
1	AA	892	A	N3-C4-N9	5.83	132.06	127.40
1	AA	1081	A	N3-C4-N9	5.83	132.06	127.40
1	AA	1117	A	C4-C5-C6	5.83	119.91	117.00
22	AV	21	A	N3-C4-N9	5.83	132.06	127.40
26	BA	502	A	N3-C4-N9	5.83	132.06	127.40
26	BA	621	A	N9-C4-C5	5.83	108.13	105.80
26	BA	1433	A	N3-C4-N9	5.83	132.06	127.40
26	BA	1679	A	N3-C4-N9	5.83	132.06	127.40
26	BA	1713	A	C8-N9-C4	5.83	108.13	105.80
26	BA	1913	A	C8-N9-C4	5.83	108.13	105.80
26	BA	1978	A	C4-C5-C6	5.83	119.91	117.00
26	BA	2147	A	C4-C5-C6	5.83	119.91	117.00
26	BA	2835	A	N3-C4-N9	5.83	132.06	127.40
1	AA	155	A	N3-C4-N9	5.83	132.06	127.40
26	BA	149	A	C4-C5-C6	5.83	119.91	117.00
26	BA	279	A	C4-C5-C6	5.83	119.91	117.00
26	BA	844	A	C4-C5-C6	5.83	119.91	117.00
26	BA	1819	A	N3-C4-N9	5.83	132.06	127.40
26	BA	2134	A	N3-C4-N9	5.83	132.06	127.40
26	BA	2335	A	C8-N9-C4	5.83	108.13	105.80
27	BB	29	A	N9-C4-C5	5.83	108.13	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	353	A	C4-C5-C6	5.83	119.91	117.00
1	AA	411	A	C4-C5-C6	5.83	119.91	117.00
1	AA	815	A	C8-N9-C4	5.83	108.13	105.80
1	AA	975	A	N3-C4-N9	5.83	132.06	127.40
1	AA	996	A	C4-C5-C6	5.83	119.91	117.00
1	AA	1410	A	C4-C5-C6	5.83	119.91	117.00
23	AW	14	A	N3-C4-N9	5.83	132.06	127.40
23	AW	31	A	C4-C5-C6	5.83	119.91	117.00
26	BA	118	A	N3-C4-N9	5.83	132.06	127.40
26	BA	655	A	C4-C5-C6	5.83	119.91	117.00
26	BA	804	A	N3-C4-N9	5.83	132.06	127.40
26	BA	1067	A	N3-C4-N9	5.83	132.06	127.40
26	BA	1080	A	N3-C4-N9	5.83	132.06	127.40
26	BA	1772	A	C4-C5-N7	-5.83	107.79	110.70
26	BA	1802	A	N3-C4-N9	5.83	132.06	127.40
26	BA	1981	A	N9-C4-C5	5.83	108.13	105.80
26	BA	2052	A	N3-C4-N9	5.83	132.06	127.40
26	BA	2314	A	C4-C5-C6	5.83	119.91	117.00
26	BA	2761	A	C4-C5-C6	5.83	119.91	117.00
1	AA	465	A	N3-C4-N9	5.82	132.06	127.40
1	AA	702	A	N3-C4-N9	5.82	132.06	127.40
1	AA	878	A	C4-C5-C6	5.82	119.91	117.00
1	AA	1105	A	N3-C4-N9	5.82	132.06	127.40
23	AW	14	A	C8-N9-C4	5.82	108.13	105.80
26	BA	603	A	N3-C4-N9	5.82	132.06	127.40
26	BA	609	A	N3-C4-N9	5.82	132.06	127.40
26	BA	627	A	C4-C5-C6	5.82	119.91	117.00
26	BA	1084	A	N3-C4-N9	5.82	132.06	127.40
26	BA	1378	A	C4-C5-N7	-5.82	107.79	110.70
26	BA	1757	A	N3-C4-N9	5.82	132.06	127.40
26	BA	2126	A	N3-C4-N9	5.82	132.06	127.40
26	BA	2670	A	N3-C4-N9	5.82	132.06	127.40
26	BA	2679	A	C8-N9-C4	5.82	108.13	105.80
26	BA	2711	A	N3-C4-N9	5.82	132.06	127.40
26	BA	2781	A	N3-C4-N9	5.82	132.06	127.40
26	BA	2860	A	N3-C4-N9	5.82	132.06	127.40
1	AA	199	A	N3-C4-N9	5.82	132.06	127.40
1	AA	768	A	N3-C4-N9	5.82	132.06	127.40
1	AA	794	A	N3-C4-N9	5.82	132.06	127.40
26	BA	217	A	N3-C4-N9	5.82	132.06	127.40
26	BA	508	A	C4-C5-C6	5.82	119.91	117.00
26	BA	734	A	N3-C4-N9	5.82	132.06	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1089	A	N3-C4-N9	5.82	132.06	127.40
26	BA	2482	A	N3-C4-N9	5.82	132.06	127.40
1	AA	715	A	N3-C4-N9	5.82	132.06	127.40
1	AA	759	A	C4-C5-C6	5.82	119.91	117.00
1	AA	1014	A	N3-C4-N9	5.82	132.06	127.40
25	AY	73	A	N3-C4-N9	5.82	132.06	127.40
26	BA	603	A	C8-N9-C4	5.82	108.13	105.80
26	BA	1247	A	N3-C4-N9	5.82	132.06	127.40
26	BA	1285	A	C4-C5-C6	5.82	119.91	117.00
26	BA	1654	A	N3-C4-N9	5.82	132.06	127.40
26	BA	1739	A	C4-C5-C6	5.82	119.91	117.00
26	BA	1815	A	C4-C5-C6	5.82	119.91	117.00
26	BA	2108	A	C4-C5-C6	5.82	119.91	117.00
26	BA	2198	A	N3-C4-N9	5.82	132.06	127.40
26	BA	2381	A	C4-C5-C6	5.82	119.91	117.00
26	BA	2534	A	C4-C5-C6	5.82	119.91	117.00
26	BA	2761	A	C4-C5-N7	-5.82	107.79	110.70
1	AA	441	A	N3-C4-N9	5.82	132.06	127.40
1	AA	1046	A	N3-C4-N9	5.82	132.06	127.40
26	BA	497	A	C8-N9-C4	5.82	108.13	105.80
26	BA	590	A	N3-C4-N9	5.82	132.06	127.40
26	BA	892	A	N3-C4-N9	5.82	132.06	127.40
26	BA	1640	A	N3-C4-N9	5.82	132.06	127.40
26	BA	2119	A	N3-C4-N9	5.82	132.06	127.40
26	BA	2340	A	N3-C4-N9	5.82	132.06	127.40
1	AA	197	A	C8-N9-C4	5.82	108.13	105.80
1	AA	1019	A	N3-C4-N9	5.82	132.05	127.40
1	AA	1250	A	C4-C5-C6	5.82	119.91	117.00
26	BA	265	A	C8-N9-C4	5.82	108.13	105.80
26	BA	300	A	C4-C5-C6	5.82	119.91	117.00
26	BA	761	A	C4-C5-C6	5.82	119.91	117.00
26	BA	1759	A	N3-C4-N9	5.82	132.05	127.40
26	BA	2247	A	C4-C5-C6	5.82	119.91	117.00
26	BA	2418	A	N9-C4-C5	5.82	108.13	105.80
26	BA	2513	A	C4-C5-C6	5.82	119.91	117.00
1	AA	282	A	N3-C4-N9	5.82	132.05	127.40
1	AA	415	A	N3-C4-N9	5.82	132.05	127.40
1	AA	456	A	C4-C5-C6	5.82	119.91	117.00
1	AA	777	A	N3-C4-N9	5.82	132.05	127.40
1	AA	1093	A	N3-C4-N9	5.82	132.05	127.40
1	AA	1447	A	N3-C4-N9	5.82	132.05	127.40
26	BA	626	A	N3-C4-N9	5.82	132.05	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1525	A	N3-C4-N9	5.82	132.05	127.40
26	BA	1655	A	C4-C5-C6	5.82	119.91	117.00
26	BA	1677	A	N3-C4-N9	5.82	132.05	127.40
26	BA	2893	A	C8-N9-C4	5.82	108.13	105.80
27	BB	34	A	N9-C4-C5	5.82	108.13	105.80
1	AA	130	A	C4-C5-C6	5.81	119.91	117.00
1	AA	1012	A	N3-C4-N9	5.81	132.05	127.40
26	BA	199	A	N3-C4-N9	5.81	132.05	127.40
26	BA	1077	A	C8-N9-C4	5.81	108.13	105.80
26	BA	1735	A	N3-C4-N9	5.81	132.05	127.40
26	BA	1794	A	C4-C5-C6	5.81	119.91	117.00
26	BA	1918	A	C4-C5-C6	5.81	119.91	117.00
26	BA	1966	A	C4-C5-C6	5.81	119.91	117.00
1	AA	66	A	C8-N9-C4	5.81	108.12	105.80
1	AA	655	A	N3-C4-N9	5.81	132.05	127.40
1	AA	792	A	N3-C4-N9	5.81	132.05	127.40
26	BA	155	A	C4-C5-C6	5.81	119.91	117.00
26	BA	574	A	C8-N9-C4	5.81	108.12	105.80
26	BA	749	A	C4-C5-C6	5.81	119.91	117.00
26	BA	1020	A	N3-C4-N9	5.81	132.05	127.40
26	BA	1342	A	C4-C5-C6	5.81	119.91	117.00
26	BA	1439	A	N3-C4-N9	5.81	132.05	127.40
26	BA	2376	A	N3-C4-N9	5.81	132.05	127.40
26	BA	2377	A	C8-N9-C4	5.81	108.12	105.80
1	AA	72	A	C8-N9-C4	5.81	108.12	105.80
1	AA	781	A	C8-N9-C4	5.81	108.12	105.80
26	BA	483	A	N3-C4-N9	5.81	132.05	127.40
26	BA	538	A	C4-C5-C6	5.81	119.91	117.00
26	BA	1713	A	C4-C5-C6	5.81	119.91	117.00
26	BA	1916	A	C4-C5-C6	5.81	119.91	117.00
26	BA	2278	A	N3-C4-N9	5.81	132.05	127.40
1	AA	243	A	C4-C5-C6	5.81	119.91	117.00
1	AA	253	A	C4-C5-C6	5.81	119.91	117.00
1	AA	366	A	C8-N9-C4	5.81	108.12	105.80
1	AA	602	A	C8-N9-C4	5.81	108.12	105.80
1	AA	1179	A	N3-C4-N9	5.81	132.05	127.40
23	AW	9	A	N3-C4-N9	5.81	132.05	127.40
23	AW	51	A	C4-C5-C6	5.81	119.91	117.00
26	BA	528	A	N9-C4-C5	5.81	108.12	105.80
26	BA	829	A	C8-N9-C4	5.81	108.12	105.80
26	BA	1609	A	N3-C4-N9	5.81	132.05	127.40
26	BA	1739	A	N3-C4-N9	5.81	132.05	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1854	A	C4-C5-C6	5.81	119.91	117.00
26	BA	2059	A	C4-C5-C6	5.81	119.91	117.00
26	BA	2309	A	N3-C4-N9	5.81	132.05	127.40
26	BA	2750	A	N3-C4-N9	5.81	132.05	127.40
26	BA	2814	A	C4-C5-C6	5.81	119.90	117.00
26	BA	2826	A	N3-C4-N9	5.81	132.05	127.40
1	AA	2	A	N3-C4-N9	5.81	132.04	127.40
1	AA	32	A	C8-N9-C4	5.81	108.12	105.80
1	AA	718	A	N3-C4-N9	5.81	132.05	127.40
1	AA	1248	A	C4-C5-N7	-5.81	107.80	110.70
26	BA	104	A	N3-C4-N9	5.81	132.05	127.40
26	BA	575	A	N3-C4-N9	5.81	132.05	127.40
26	BA	637	A	N3-C4-N9	5.81	132.05	127.40
26	BA	677	A	C4-C5-C6	5.81	119.90	117.00
26	BA	1509	A	C8-N9-C4	5.81	108.12	105.80
26	BA	1677	A	C8-N9-C4	5.81	108.12	105.80
26	BA	1705	A	C4-C5-C6	5.81	119.90	117.00
26	BA	1780	A	N3-C4-N9	5.81	132.05	127.40
26	BA	1791	A	N3-C4-N9	5.81	132.04	127.40
26	BA	2800	A	C8-N9-C4	5.81	108.12	105.80
27	BB	52	A	C8-N9-C4	5.81	108.12	105.80
1	AA	7	A	N3-C4-N9	5.81	132.04	127.40
1	AA	1518	A	N3-C4-N9	5.81	132.04	127.40
26	BA	83	A	C8-N9-C4	5.81	108.12	105.80
26	BA	2322	A	C4-C5-N7	-5.81	107.80	110.70
26	BA	2358	A	C4-C5-C6	5.81	119.90	117.00
26	BA	2851	A	C8-N9-C4	5.81	108.12	105.80
27	BB	34	A	C4-C5-N7	-5.81	107.80	110.70
1	AA	583	A	C8-N9-C4	5.80	108.12	105.80
1	AA	959	A	N3-C4-N9	5.80	132.04	127.40
1	AA	1271	A	N3-C4-N9	5.80	132.04	127.40
24	AX	9	A	C4-C5-C6	5.80	119.90	117.00
26	BA	270	A	N3-C4-N9	5.80	132.04	127.40
26	BA	439	A	C8-N9-C4	5.80	108.12	105.80
26	BA	721	A	N3-C4-N9	5.80	132.04	127.40
26	BA	802	A	C4-C5-C6	5.80	119.90	117.00
26	BA	918	A	C4-C5-C6	5.80	119.90	117.00
26	BA	945	A	C4-C5-C6	5.80	119.90	117.00
26	BA	1504	A	C8-N9-C4	5.80	108.12	105.80
26	BA	1508	A	N3-C4-N9	5.80	132.04	127.40
1	AA	101	A	C8-N9-C4	5.80	108.12	105.80
1	AA	974	A	C4-C5-C6	5.80	119.90	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	978	A	C4-C5-C6	5.80	119.90	117.00
1	AA	451	A	C8-N9-C4	5.80	108.12	105.80
1	AA	815	A	N3-C4-N9	5.80	132.04	127.40
1	AA	1256	A	N3-C4-N9	5.80	132.04	127.40
26	BA	821	A	N3-C4-N9	5.80	132.04	127.40
26	BA	900	A	C4-C5-C6	5.80	119.90	117.00
26	BA	1772	A	N9-C4-C5	5.80	108.12	105.80
26	BA	2176	A	C4-C5-C6	5.80	119.90	117.00
26	BA	2899	A	N3-C4-N9	5.80	132.04	127.40
1	AA	466	A	N3-C4-N9	5.80	132.04	127.40
1	AA	1492	A	C4-C5-C6	5.80	119.90	117.00
26	BA	391	A	C8-N9-C4	5.80	108.12	105.80
26	BA	750	A	C8-N9-C4	5.80	108.12	105.80
26	BA	1040	A	N9-C4-C5	5.80	108.12	105.80
26	BA	1717	A	C8-N9-C4	5.80	108.12	105.80
26	BA	2003	A	C8-N9-C4	5.80	108.12	105.80
26	BA	2020	A	N3-C4-N9	5.80	132.04	127.40
26	BA	2090	A	C4-C5-C6	5.80	119.90	117.00
27	BB	66	A	C8-N9-C4	5.80	108.12	105.80
1	AA	179	A	C4-C5-C6	5.80	119.90	117.00
1	AA	246	A	C8-N9-C4	5.80	108.12	105.80
1	AA	1101	A	N3-C4-N9	5.80	132.04	127.40
23	AW	66	A	N3-C4-N9	5.80	132.04	127.40
26	BA	513	A	C8-N9-C4	5.80	108.12	105.80
26	BA	1749	A	N3-C4-N9	5.80	132.04	127.40
1	AA	315	A	C8-N9-C4	5.80	108.12	105.80
1	AA	1111	A	N3-C4-N9	5.80	132.04	127.40
1	AA	1248	A	C4-C5-C6	5.80	119.90	117.00
1	AA	1257	A	C4-C5-C6	5.80	119.90	117.00
1	AA	1493	A	C4-C5-C6	5.80	119.90	117.00
25	AY	38	A	C4-C5-C6	5.80	119.90	117.00
26	BA	1165	A	C4-C5-C6	5.80	119.90	117.00
26	BA	1274	A	N3-C4-N9	5.80	132.04	127.40
26	BA	1626	A	N3-C4-N9	5.80	132.04	127.40
26	BA	2052	A	C4-C5-C6	5.80	119.90	117.00
1	AA	535	A	N3-C4-N9	5.79	132.04	127.40
1	AA	996	A	N3-C4-N9	5.79	132.04	127.40
24	AX	58	A	N3-C4-N9	5.79	132.04	127.40
25	AY	38	A	N3-C4-N9	5.79	132.04	127.40
25	AY	73	A	C4-C5-C6	5.79	119.90	117.00
26	BA	1080	A	C8-N9-C4	5.79	108.12	105.80
26	BA	1569	A	N3-C4-N9	5.79	132.04	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1678	A	C8-N9-C4	5.79	108.12	105.80
1	AA	246	A	C4-C5-C6	5.79	119.90	117.00
1	AA	279	A	C8-N9-C4	5.79	108.12	105.80
1	AA	1150	A	N9-C4-C5	5.79	108.12	105.80
22	AV	15	A	C8-N9-C4	5.79	108.12	105.80
26	BA	1275	A	C4-C5-C6	5.79	119.90	117.00
26	BA	1275	A	C8-N9-C4	5.79	108.12	105.80
26	BA	1700	A	N3-C4-N9	5.79	132.03	127.40
26	BA	1932	A	C4-C5-C6	5.79	119.90	117.00
26	BA	2037	A	C4-C5-C6	5.79	119.90	117.00
26	BA	2778	A	C8-N9-C4	5.79	108.12	105.80
26	BA	19	A	N3-C4-N9	5.79	132.03	127.40
26	BA	89	A	C4-C5-C6	5.79	119.90	117.00
26	BA	244	A	C4-C5-C6	5.79	119.89	117.00
26	BA	478	A	N3-C4-N9	5.79	132.03	127.40
26	BA	507	A	N3-C4-N9	5.79	132.03	127.40
26	BA	1133	A	N3-C4-N9	5.79	132.03	127.40
26	BA	1470	A	C8-N9-C4	5.79	108.12	105.80
26	BA	1652	A	C8-N9-C4	5.79	108.12	105.80
26	BA	1978	A	N3-C4-N9	5.79	132.03	127.40
26	BA	2270	A	N3-C4-N9	5.79	132.03	127.40
26	BA	2654	A	C8-N9-C4	5.79	108.12	105.80
26	BA	2829	A	C8-N9-C4	5.79	108.12	105.80
1	AA	816	A	N3-C4-N9	5.79	132.03	127.40
1	AA	1480	A	N3-C4-N9	5.79	132.03	127.40
26	BA	739	A	N3-C4-N9	5.79	132.03	127.40
26	BA	1969	A	C8-N9-C4	5.79	108.12	105.80
26	BA	2572	A	N3-C4-N9	5.79	132.03	127.40
26	BA	2726	A	C4-C5-C6	5.79	119.89	117.00
1	AA	946	A	C8-N9-C4	5.79	108.12	105.80
1	AA	1269	A	N3-C4-N9	5.79	132.03	127.40
26	BA	223	A	C4-C5-C6	5.79	119.89	117.00
26	BA	563	A	N3-C4-N9	5.79	132.03	127.40
26	BA	761	A	N3-C4-N9	5.79	132.03	127.40
26	BA	899	A	N3-C4-N9	5.79	132.03	127.40
26	BA	1551	A	N3-C4-N9	5.79	132.03	127.40
26	BA	1552	A	N3-C4-N9	5.79	132.03	127.40
26	BA	1987	A	C4-C5-C6	5.79	119.89	117.00
26	BA	2835	A	C8-N9-C4	5.79	108.11	105.80
1	AA	131	A	C4-C5-N7	-5.79	107.81	110.70
1	AA	274	A	N3-C4-N9	5.79	132.03	127.40
1	AA	389	A	C4-C5-C6	5.79	119.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	58	A	C8-N9-C4	5.79	108.11	105.80
26	BA	213	A	N3-C4-N9	5.79	132.03	127.40
26	BA	1912	A	N3-C4-N9	5.79	132.03	127.40
26	BA	2589	A	N9-C4-C5	5.79	108.11	105.80
1	AA	338	A	C8-N9-C4	5.79	108.11	105.80
1	AA	673	A	N3-C4-N9	5.79	132.03	127.40
1	AA	1016	A	N3-C4-N9	5.79	132.03	127.40
1	AA	1101	A	C8-N9-C4	5.79	108.11	105.80
23	AW	41	A	C4-C5-N7	-5.79	107.81	110.70
26	BA	320	A	C8-N9-C4	5.79	108.11	105.80
26	BA	460	A	C4-C5-C6	5.79	119.89	117.00
26	BA	526	A	C4-C5-C6	5.79	119.89	117.00
26	BA	1226	A	N3-C4-N9	5.79	132.03	127.40
26	BA	1789	A	N3-C4-N9	5.79	132.03	127.40
26	BA	1815	A	C8-N9-C4	5.79	108.11	105.80
1	AA	28	A	C8-N9-C4	5.78	108.11	105.80
1	AA	1196	A	N3-C4-N9	5.78	132.03	127.40
1	AA	1287	A	N3-C4-N9	5.78	132.03	127.40
26	BA	272	A	C8-N9-C4	5.78	108.11	105.80
26	BA	514	A	N9-C4-C5	5.78	108.11	105.80
26	BA	1308	A	N9-C4-C5	5.78	108.11	105.80
26	BA	1655	A	N3-C4-N9	5.78	132.03	127.40
26	BA	1784	A	C8-N9-C4	5.78	108.11	105.80
26	BA	1786	A	C4-C5-C6	5.78	119.89	117.00
26	BA	1794	A	C8-N9-C4	5.78	108.11	105.80
26	BA	2281	A	C8-N9-C4	5.78	108.11	105.80
27	BB	29	A	N3-C4-N9	5.78	132.03	127.40
26	BA	821	A	C4-C5-C6	5.78	119.89	117.00
26	BA	941	A	C4-C5-C6	5.78	119.89	117.00
26	BA	1308	A	C4-C5-C6	5.78	119.89	117.00
26	BA	2013	A	C8-N9-C4	5.78	108.11	105.80
1	AA	288	A	N3-C4-N9	5.78	132.02	127.40
1	AA	411	A	N9-C4-C5	5.78	108.11	105.80
25	AY	26	A	C8-N9-C4	5.78	108.11	105.80
26	BA	608	A	C8-N9-C4	5.78	108.11	105.80
26	BA	764	A	C8-N9-C4	5.78	108.11	105.80
26	BA	1073	A	N3-C4-N9	5.78	132.03	127.40
26	BA	1630	A	C4-C5-N7	-5.78	107.81	110.70
26	BA	1808	A	N3-C4-N9	5.78	132.02	127.40
26	BA	1854	A	N3-C4-N9	5.78	132.02	127.40
26	BA	2225	A	N9-C4-C5	5.78	108.11	105.80
26	BA	2565	A	C4-C5-C6	5.78	119.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2682	A	N3-C4-N9	5.78	132.03	127.40
26	BA	2734	A	C4-C5-C6	5.78	119.89	117.00
26	BA	2820	A	N3-C4-N9	5.78	132.03	127.40
1	AA	415	A	C4-C5-C6	5.78	119.89	117.00
1	AA	749	A	N3-C4-N9	5.78	132.02	127.40
1	AA	1441	A	N3-C4-N9	5.78	132.02	127.40
26	BA	111	A	N3-C4-N9	5.78	132.02	127.40
26	BA	2031	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1225	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1285	A	N3-C4-N9	5.78	132.02	127.40
26	BA	126	A	N3-C4-N9	5.78	132.02	127.40
26	BA	508	A	N3-C4-N9	5.78	132.02	127.40
26	BA	829	A	N3-C4-N9	5.78	132.02	127.40
26	BA	1008	A	C8-N9-C4	5.78	108.11	105.80
26	BA	1142	A	C8-N9-C4	5.78	108.11	105.80
26	BA	1431	A	C8-N9-C4	5.78	108.11	105.80
26	BA	2503	A	N3-C4-N9	5.78	132.02	127.40
26	BA	2753	A	N3-C4-N9	5.78	132.02	127.40
1	AA	374	A	N3-C4-N9	5.78	132.02	127.40
1	AA	1311	A	N3-C4-N9	5.78	132.02	127.40
26	BA	167	A	N3-C4-N9	5.78	132.02	127.40
26	BA	677	A	N3-C4-N9	5.78	132.02	127.40
26	BA	1069	A	N3-C4-N9	5.78	132.02	127.40
26	BA	1690	A	N3-C4-N9	5.78	132.02	127.40
26	BA	1749	A	C4-C5-C6	5.78	119.89	117.00
26	BA	1918	A	N3-C4-N9	5.78	132.02	127.40
26	BA	1932	A	N3-C4-N9	5.78	132.02	127.40
1	AA	101	A	N3-C4-N9	5.77	132.02	127.40
1	AA	393	A	N9-C4-C5	5.77	108.11	105.80
1	AA	978	A	C8-N9-C4	5.77	108.11	105.80
26	BA	984	A	N3-C4-N9	5.77	132.02	127.40
26	BA	1057	A	C4-C5-C6	5.77	119.89	117.00
26	BA	1342	A	N3-C4-N9	5.77	132.02	127.40
26	BA	1876	A	N9-C4-C5	5.77	108.11	105.80
26	BA	2135	A	C8-N9-C4	5.77	108.11	105.80
1	AA	44	A	N9-C4-C5	5.77	108.11	105.80
1	AA	50	A	N3-C4-N9	5.77	132.02	127.40
1	AA	675	A	C8-N9-C4	5.77	108.11	105.80
1	AA	759	A	N3-C4-N9	5.77	132.02	127.40
1	AA	889	A	N9-C4-C5	5.77	108.11	105.80
24	AX	9	A	N3-C4-N9	5.77	132.02	127.40
26	BA	42	A	C8-N9-C4	5.77	108.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	83	A	C4-C5-C6	5.77	119.89	117.00
26	BA	125	A	N3-C4-N9	5.77	132.02	127.40
26	BA	422	A	N3-C4-N9	5.77	132.02	127.40
26	BA	627	A	N3-C4-N9	5.77	132.02	127.40
26	BA	825	A	C4-C5-N7	-5.77	107.81	110.70
26	BA	1420	A	N3-C4-N9	5.77	132.02	127.40
26	BA	1654	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2054	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2119	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2169	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2358	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2503	A	C4-C5-C6	5.77	119.89	117.00
26	BA	2589	A	C4-C5-N7	-5.77	107.81	110.70
26	BA	2679	A	N3-C4-N9	5.77	132.02	127.40
1	AA	1288	A	N3-C4-N9	5.77	132.02	127.40
26	BA	1848	A	N3-C4-N9	5.77	132.02	127.40
1	AA	238	A	N3-C4-N9	5.77	132.01	127.40
1	AA	535	A	C8-N9-C4	5.77	108.11	105.80
1	AA	673	A	C8-N9-C4	5.77	108.11	105.80
1	AA	975	A	C8-N9-C4	5.77	108.11	105.80
23	AW	41	A	N3-C4-N9	5.77	132.01	127.40
25	AY	35	A	C8-N9-C4	5.77	108.11	105.80
26	BA	609	A	C8-N9-C4	5.77	108.11	105.80
26	BA	1359	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2108	A	N9-C4-C5	5.77	108.11	105.80
26	BA	2358	A	N3-C4-N9	5.77	132.01	127.40
26	BA	2590	A	C4-C5-C6	5.77	119.88	117.00
26	BA	2614	A	N3-C4-N9	5.77	132.02	127.40
26	BA	2675	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2725	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2882	A	N3-C4-N9	5.77	132.02	127.40
1	AA	430	A	N3-C4-N9	5.77	132.01	127.40
26	BA	125	A	C8-N9-C4	5.77	108.11	105.80
26	BA	1413	A	N3-C4-N9	5.77	132.01	127.40
26	BA	2015	A	N3-C4-N9	5.77	132.01	127.40
26	BA	2033	A	C4-C5-N7	-5.77	107.82	110.70
26	BA	2037	A	N3-C4-N9	5.77	132.01	127.40
26	BA	2059	A	N3-C4-N9	5.77	132.01	127.40
26	BA	2503	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2530	A	N3-C4-N9	5.77	132.01	127.40
26	BA	2560	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2614	A	C4-C5-C6	5.77	119.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BB	46	A	N3-C4-N9	5.77	132.01	127.40
1	AA	78	A	N3-C4-N9	5.77	132.01	127.40
1	AA	782	A	N9-C4-C5	5.77	108.11	105.80
1	AA	1179	A	C8-N9-C4	5.77	108.11	105.80
1	AA	1204	A	N3-C4-N9	5.77	132.01	127.40
26	BA	412	A	C8-N9-C4	5.77	108.11	105.80
26	BA	480	A	C4-C5-C6	5.77	119.88	117.00
26	BA	781	A	N3-C4-N9	5.77	132.01	127.40
26	BA	1134	A	C8-N9-C4	5.77	108.11	105.80
26	BA	2434	A	N3-C4-N9	5.77	132.01	127.40
26	BA	2726	A	C8-N9-C4	5.77	108.11	105.80
1	AA	364	A	N3-C4-N9	5.76	132.01	127.40
1	AA	459	A	N3-C4-N9	5.76	132.01	127.40
26	BA	221	A	C8-N9-C4	5.76	108.11	105.80
26	BA	507	A	C8-N9-C4	5.76	108.11	105.80
26	BA	927	A	N3-C4-N9	5.76	132.01	127.40
26	BA	1014	A	C4-C5-N7	-5.76	107.82	110.70
26	BA	1265	A	N3-C4-N9	5.76	132.01	127.40
26	BA	1286	A	C4-C5-C6	5.76	119.88	117.00
1	AA	499	A	C4-C5-N7	-5.76	107.82	110.70
1	AA	749	A	C8-N9-C4	5.76	108.11	105.80
26	BA	49	A	C8-N9-C4	5.76	108.11	105.80
26	BA	262	A	N3-C4-N9	5.76	132.01	127.40
26	BA	340	A	C4-C5-C6	5.76	119.88	117.00
26	BA	655	A	N3-C4-N9	5.76	132.01	127.40
26	BA	1698	A	C8-N9-C4	5.76	108.11	105.80
26	BA	2453	A	N3-C4-N9	5.76	132.01	127.40
26	BA	2758	A	C8-N9-C4	5.76	108.11	105.80
1	AA	243	A	N9-C4-C5	5.76	108.10	105.80
1	AA	602	A	C4-C5-C6	5.76	119.88	117.00
1	AA	729	A	N3-C4-N9	5.76	132.01	127.40
1	AA	1280	A	C8-N9-C4	5.76	108.10	105.80
25	AY	9	A	C8-N9-C4	5.76	108.11	105.80
26	BA	311	A	C4-C5-C6	5.76	119.88	117.00
26	BA	1046	A	C8-N9-C4	5.76	108.10	105.80
26	BA	1872	A	N3-C4-N9	5.76	132.01	127.40
26	BA	2070	A	N3-C4-N9	5.76	132.01	127.40
26	BA	2266	A	C4-C5-C6	5.76	119.88	117.00
1	AA	50	A	C8-N9-C4	5.76	108.10	105.80
1	AA	143	A	N3-C4-N9	5.76	132.01	127.40
1	AA	151	A	C4-C5-N7	-5.76	107.82	110.70
1	AA	321	A	C8-N9-C4	5.76	108.10	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	935	A	C8-N9-C4	5.76	108.10	105.80
1	AA	958	A	N3-C4-N9	5.76	132.01	127.40
22	AV	15	A	N3-C4-N9	5.76	132.01	127.40
26	BA	167	A	C8-N9-C4	5.76	108.10	105.80
26	BA	699	A	N3-C4-N9	5.76	132.01	127.40
26	BA	911	A	N3-C4-N9	5.76	132.01	127.40
26	BA	1077	A	N3-C4-N9	5.76	132.01	127.40
26	BA	1630	A	N9-C4-C5	5.76	108.10	105.80
26	BA	2738	A	C8-N9-C4	5.76	108.10	105.80
1	AA	383	A	N3-C4-N9	5.76	132.01	127.40
1	AA	495	A	C4-C5-C6	5.76	119.88	117.00
1	AA	583	A	N3-C4-N9	5.76	132.01	127.40
26	BA	1077	A	C4-C5-C6	5.76	119.88	117.00
26	BA	1690	A	C4-C5-C6	5.76	119.88	117.00
26	BA	1700	A	C8-N9-C4	5.76	108.10	105.80
26	BA	1786	A	N3-C4-N9	5.76	132.01	127.40
26	BA	1858	A	C8-N9-C4	5.76	108.10	105.80
26	BA	2183	A	N3-C4-N9	5.76	132.01	127.40
26	BA	2322	A	C8-N9-C4	5.76	108.10	105.80
1	AA	152	A	N3-C4-N9	5.76	132.00	127.40
1	AA	996	A	C8-N9-C4	5.76	108.10	105.80
1	AA	1246	A	C4-C5-C6	5.76	119.88	117.00
1	AA	1502	A	C8-N9-C4	5.76	108.10	105.80
26	BA	320	A	C4-C5-C6	5.76	119.88	117.00
26	BA	340	A	C8-N9-C4	5.76	108.10	105.80
26	BA	346	A	C8-N9-C4	5.76	108.10	105.80
26	BA	515	A	N3-C4-N9	5.76	132.01	127.40
26	BA	676	A	C4-C5-C6	5.76	119.88	117.00
26	BA	844	A	N3-C4-N9	5.76	132.00	127.40
26	BA	1254	A	N3-C4-N9	5.76	132.00	127.40
26	BA	1393	A	N3-C4-N9	5.76	132.00	127.40
26	BA	1419	A	N9-C4-C5	5.76	108.10	105.80
26	BA	1919	A	C8-N9-C4	5.76	108.10	105.80
26	BA	2247	A	C8-N9-C4	5.76	108.10	105.80
26	BA	2541	A	C8-N9-C4	5.76	108.10	105.80
1	AA	243	A	C4-C5-N7	-5.75	107.82	110.70
1	AA	411	A	C4-C5-N7	-5.75	107.82	110.70
26	BA	1689	A	N3-C4-N9	5.75	132.00	127.40
26	BA	2288	A	N3-C4-N9	5.75	132.00	127.40
1	AA	181	A	C8-N9-C4	5.75	108.10	105.80
1	AA	298	A	N3-C4-N9	5.75	132.00	127.40
1	AA	694	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	1216	A	N3-C4-N9	5.75	132.00	127.40
26	BA	1010	A	N3-C4-N9	5.75	132.00	127.40
26	BA	1502	A	N3-C4-N9	5.75	132.00	127.40
26	BA	1580	A	C8-N9-C4	5.75	108.10	105.80
26	BA	1616	A	N3-C4-N9	5.75	132.00	127.40
26	BA	1815	A	N3-C4-N9	5.75	132.00	127.40
26	BA	1890	A	C8-N9-C4	5.75	108.10	105.80
26	BA	1916	A	N3-C4-N9	5.75	132.00	127.40
26	BA	2534	A	N3-C4-N9	5.75	132.00	127.40
27	BB	104	A	N3-C4-N9	5.75	132.00	127.40
1	AA	195	A	N9-C4-C5	5.75	108.10	105.80
1	AA	414	A	C8-N9-C4	5.75	108.10	105.80
1	AA	493	A	C4-C5-C6	5.75	119.88	117.00
1	AA	767	A	N3-C4-N9	5.75	132.00	127.40
26	BA	947	A	N3-C4-N9	5.75	132.00	127.40
26	BA	2577	A	N3-C4-N9	5.75	132.00	127.40
1	AA	44	A	C4-C5-N7	-5.75	107.83	110.70
1	AA	873	A	C8-N9-C4	5.75	108.10	105.80
26	BA	244	A	N3-C4-N9	5.75	132.00	127.40
26	BA	1532	A	C8-N9-C4	5.75	108.10	105.80
26	BA	1705	A	C8-N9-C4	5.75	108.10	105.80
26	BA	2058	A	N3-C4-N9	5.75	132.00	127.40
26	BA	2095	A	C8-N9-C4	5.75	108.10	105.80
26	BA	2388	A	C4-C5-C6	5.75	119.88	117.00
27	BB	78	A	C4-C5-N7	-5.75	107.83	110.70
1	AA	554	A	C4-C5-C6	5.75	119.87	117.00
1	AA	573	A	N3-C4-N9	5.75	132.00	127.40
1	AA	649	A	N3-C4-N9	5.75	132.00	127.40
1	AA	1042	A	N3-C4-N9	5.75	132.00	127.40
1	AA	1081	A	C8-N9-C4	5.75	108.10	105.80
1	AA	1229	A	N3-C4-N9	5.75	132.00	127.40
1	AA	1396	A	C8-N9-C4	5.75	108.10	105.80
26	BA	279	A	C8-N9-C4	5.75	108.10	105.80
26	BA	311	A	N3-C4-N9	5.75	132.00	127.40
26	BA	322	A	N3-C4-N9	5.75	132.00	127.40
26	BA	905	A	C4-C5-N7	-5.75	107.83	110.70
26	BA	1503	A	N3-C4-N9	5.75	132.00	127.40
26	BA	1786	A	C8-N9-C4	5.75	108.10	105.80
26	BA	1853	A	N3-C4-N9	5.75	132.00	127.40
26	BA	2019	A	N9-C4-C5	5.75	108.10	105.80
26	BA	2030	A	N3-C4-N9	5.75	132.00	127.40
26	BA	2101	A	N3-C4-N9	5.75	132.00	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2602	A	C8-N9-C4	5.75	108.10	105.80
26	BA	2665	A	C8-N9-C4	5.75	108.10	105.80
1	AA	728	A	N3-C4-N9	5.75	132.00	127.40
1	AA	1102	A	C8-N9-C4	5.75	108.10	105.80
1	AA	1500	A	C8-N9-C4	5.75	108.10	105.80
23	AW	51	A	C8-N9-C4	5.75	108.10	105.80
26	BA	53	A	N9-C4-C5	5.75	108.10	105.80
26	BA	221	A	C4-C5-C6	5.75	119.87	117.00
26	BA	294	A	N9-C4-C5	5.75	108.10	105.80
26	BA	482	A	C8-N9-C4	5.75	108.10	105.80
26	BA	825	A	N3-C4-N9	5.75	132.00	127.40
26	BA	1237	A	C8-N9-C4	5.75	108.10	105.80
26	BA	1304	A	C4-C5-N7	-5.75	107.83	110.70
26	BA	2311	A	C8-N9-C4	5.75	108.10	105.80
26	BA	149	A	N3-C4-N9	5.75	132.00	127.40
26	BA	575	A	C8-N9-C4	5.75	108.10	105.80
26	BA	788	A	C8-N9-C4	5.75	108.10	105.80
26	BA	973	A	C8-N9-C4	5.75	108.10	105.80
1	AA	315	A	N3-C4-N9	5.74	132.00	127.40
1	AA	1082	A	C8-N9-C4	5.74	108.10	105.80
1	AA	1170	A	N9-C4-C5	5.74	108.10	105.80
1	AA	1188	A	C8-N9-C4	5.74	108.10	105.80
1	AA	1368	A	C4-C5-N7	-5.74	107.83	110.70
26	BA	718	A	C8-N9-C4	5.74	108.10	105.80
26	BA	910	A	C4-C5-N7	-5.74	107.83	110.70
26	BA	945	A	N3-C4-N9	5.74	132.00	127.40
26	BA	947	A	C4-C5-C6	5.74	119.87	117.00
26	BA	1009	A	N3-C4-N9	5.74	131.99	127.40
26	BA	1322	A	C8-N9-C4	5.74	108.10	105.80
26	BA	1586	A	N3-C4-N9	5.74	131.99	127.40
26	BA	1652	A	N9-C4-C5	5.74	108.10	105.80
26	BA	1722	A	C8-N9-C4	5.74	108.10	105.80
26	BA	1755	A	C4-C5-C6	5.74	119.87	117.00
26	BA	2726	A	N3-C4-N9	5.74	132.00	127.40
1	AA	309	A	N9-C4-C5	5.74	108.10	105.80
1	AA	456	A	N3-C4-N9	5.74	131.99	127.40
1	AA	914	A	N3-C4-N9	5.74	131.99	127.40
1	AA	969	A	N3-C4-N9	5.74	131.99	127.40
22	AV	15	A	C4-C5-C6	5.74	119.87	117.00
26	BA	73	A	N3-C4-N9	5.74	131.99	127.40
26	BA	541	A	C8-N9-C4	5.74	108.10	105.80
26	BA	1515	A	C4-C5-C6	5.74	119.87	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1938	A	C8-N9-C4	5.74	108.10	105.80
26	BA	2241	A	N3-C4-N9	5.74	131.99	127.40
27	BB	119	A	C8-N9-C4	5.74	108.10	105.80
1	AA	663	A	N3-C4-N9	5.74	131.99	127.40
1	AA	687	A	C4-C5-C6	5.74	119.87	117.00
1	AA	878	A	C8-N9-C4	5.74	108.10	105.80
1	AA	1534	A	N3-C4-N9	5.74	131.99	127.40
24	AX	76	A	C8-N9-C4	5.74	108.10	105.80
26	BA	103	A	C8-N9-C4	5.74	108.10	105.80
26	BA	586	A	N3-C4-N9	5.74	131.99	127.40
26	BA	727	A	C4-C5-C6	5.74	119.87	117.00
26	BA	781	A	C8-N9-C4	5.74	108.10	105.80
26	BA	983	A	C4-C5-C6	5.74	119.87	117.00
26	BA	1050	A	C8-N9-C4	5.74	108.10	105.80
26	BA	1147	A	C8-N9-C4	5.74	108.10	105.80
26	BA	1593	A	C8-N9-C4	5.74	108.10	105.80
26	BA	1593	A	N3-C4-N9	5.74	131.99	127.40
26	BA	2590	A	C4-C5-N7	-5.74	107.83	110.70
26	BA	2738	A	N3-C4-N9	5.74	131.99	127.40
26	BA	2835	A	C4-C5-C6	5.74	119.87	117.00
1	AA	77	A	N3-C4-N9	5.74	131.99	127.40
1	AA	441	A	C4-C5-N7	-5.74	107.83	110.70
22	AV	22	A	N3-C4-N9	5.74	131.99	127.40
26	BA	324	A	C8-N9-C4	5.74	108.09	105.80
26	BA	526	A	C8-N9-C4	5.74	108.10	105.80
26	BA	1385	A	C4-C5-N7	-5.74	107.83	110.70
26	BA	1420	A	C8-N9-C4	5.74	108.10	105.80
26	BA	2126	A	C8-N9-C4	5.74	108.10	105.80
1	AA	1248	A	C8-N9-C4	5.74	108.09	105.80
26	BA	83	A	N3-C4-N9	5.74	131.99	127.40
26	BA	371	A	C8-N9-C4	5.74	108.09	105.80
26	BA	402	A	C8-N9-C4	5.74	108.09	105.80
26	BA	460	A	N3-C4-N9	5.74	131.99	127.40
26	BA	918	A	N3-C4-N9	5.74	131.99	127.40
26	BA	1254	A	C8-N9-C4	5.74	108.09	105.80
26	BA	1321	A	C8-N9-C4	5.74	108.09	105.80
26	BA	1689	A	C4-C5-C6	5.74	119.87	117.00
26	BA	1690	A	C8-N9-C4	5.74	108.09	105.80
26	BA	1937	A	C4-C5-C6	5.74	119.87	117.00
26	BA	2117	A	C8-N9-C4	5.74	108.09	105.80
1	AA	179	A	N9-C4-C5	5.74	108.09	105.80
1	AA	246	A	N3-C4-N9	5.74	131.99	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	937	A	C8-N9-C4	5.74	108.09	105.80
1	AA	1155	A	C8-N9-C4	5.74	108.09	105.80
1	AA	1447	A	C8-N9-C4	5.74	108.09	105.80
26	BA	155	A	N3-C4-N9	5.74	131.99	127.40
26	BA	223	A	N3-C4-N9	5.74	131.99	127.40
26	BA	609	A	C4-C5-C6	5.74	119.87	117.00
26	BA	1366	A	C8-N9-C4	5.74	108.09	105.80
26	BA	1522	A	C8-N9-C4	5.74	108.09	105.80
26	BA	1755	A	C8-N9-C4	5.74	108.09	105.80
26	BA	2019	A	C4-C5-C6	5.74	119.87	117.00
1	AA	1000	A	N9-C4-C5	5.73	108.09	105.80
1	AA	1413	A	C8-N9-C4	5.73	108.09	105.80
26	BA	990	A	C4-C5-C6	5.73	119.87	117.00
26	BA	1246	A	N3-C4-N9	5.73	131.99	127.40
26	BA	2336	A	C8-N9-C4	5.73	108.09	105.80
1	AA	1254	A	C8-N9-C4	5.73	108.09	105.80
1	AA	1434	A	C8-N9-C4	5.73	108.09	105.80
25	AY	69	A	C8-N9-C4	5.73	108.09	105.80
26	BA	222	A	C8-N9-C4	5.73	108.09	105.80
26	BA	1566	A	N3-C4-N9	5.73	131.99	127.40
26	BA	1641	A	N3-C4-N9	5.73	131.99	127.40
26	BA	1749	A	C8-N9-C4	5.73	108.09	105.80
26	BA	1819	A	C8-N9-C4	5.73	108.09	105.80
26	BA	1901	A	C4-C5-C6	5.73	119.87	117.00
26	BA	2147	A	N3-C4-N9	5.73	131.99	127.40
26	BA	2872	A	N3-C4-N9	5.73	131.99	127.40
27	BB	108	A	C4-C5-C6	5.73	119.87	117.00
1	AA	16	A	N3-C4-N9	5.73	131.98	127.40
1	AA	139	A	N3-C4-N9	5.73	131.99	127.40
1	AA	432	A	C4-C5-C6	5.73	119.86	117.00
1	AA	602	A	N3-C4-N9	5.73	131.99	127.40
1	AA	1150	A	C4-C5-N7	-5.73	107.83	110.70
1	AA	1289	A	C4-C5-C6	5.73	119.86	117.00
26	BA	104	A	C8-N9-C4	5.73	108.09	105.80
26	BA	788	A	N3-C4-N9	5.73	131.99	127.40
26	BA	1286	A	N3-C4-N9	5.73	131.98	127.40
26	BA	1913	A	C4-C5-C6	5.73	119.86	117.00
26	BA	2173	A	C8-N9-C4	5.73	108.09	105.80
26	BA	2314	A	N3-C4-N9	5.73	131.99	127.40
27	BB	50	A	C8-N9-C4	5.73	108.09	105.80
1	AA	10	A	N3-C4-N9	5.73	131.98	127.40
1	AA	648	A	N3-C4-N9	5.73	131.98	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1275	A	N3-C4-N9	5.73	131.98	127.40
26	BA	310	A	C4-C5-C6	5.73	119.86	117.00
26	BA	1603	A	C8-N9-C4	5.73	108.09	105.80
26	BA	1890	A	N3-C4-N9	5.73	131.98	127.40
26	BA	2031	A	N3-C4-N9	5.73	131.98	127.40
1	AA	1067	A	N3-C4-N9	5.73	131.98	127.40
1	AA	1117	A	N3-C4-N9	5.73	131.98	127.40
1	AA	1239	A	N3-C4-N9	5.73	131.98	127.40
1	AA	1248	A	N9-C4-C5	5.73	108.09	105.80
1	AA	1311	A	C4-C5-N7	-5.73	107.84	110.70
26	BA	38	A	C4-C5-C6	5.73	119.86	117.00
26	BA	477	A	N3-C4-N9	5.73	131.98	127.40
26	BA	2284	A	C8-N9-C4	5.73	108.09	105.80
26	BA	2322	A	N9-C4-C5	5.73	108.09	105.80
26	BA	2406	A	N3-C4-N9	5.73	131.98	127.40
1	AA	53	A	C8-N9-C4	5.73	108.09	105.80
1	AA	119	A	C8-N9-C4	5.73	108.09	105.80
26	BA	256	A	C8-N9-C4	5.73	108.09	105.80
26	BA	526	A	N3-C4-N9	5.73	131.98	127.40
26	BA	925	A	C8-N9-C4	5.73	108.09	105.80
26	BA	2566	A	C8-N9-C4	5.73	108.09	105.80
1	AA	263	A	N9-C4-C5	5.72	108.09	105.80
1	AA	510	A	N9-C4-C5	5.72	108.09	105.80
1	AA	1519	A	N3-C4-N9	5.72	131.98	127.40
26	BA	324	A	N3-C4-N9	5.72	131.98	127.40
26	BA	936	A	N3-C4-N9	5.72	131.98	127.40
26	BA	1705	A	N3-C4-N9	5.72	131.98	127.40
1	AA	1145	A	N3-C4-N9	5.72	131.98	127.40
1	AA	1493	A	C4-C5-N7	-5.72	107.84	110.70
26	BA	165	A	N9-C4-C5	5.72	108.09	105.80
26	BA	637	A	C8-N9-C4	5.72	108.09	105.80
26	BA	1057	A	N3-C4-N9	5.72	131.98	127.40
26	BA	1275	A	N3-C4-N9	5.72	131.98	127.40
26	BA	1803	A	N9-C4-C5	5.72	108.09	105.80
26	BA	2448	A	C4-C5-C6	5.72	119.86	117.00
27	BB	34	A	C8-N9-C4	5.72	108.09	105.80
27	BB	108	A	N3-C4-N9	5.72	131.98	127.40
1	AA	44	A	C4-C5-C6	5.72	119.86	117.00
1	AA	329	A	C8-N9-C4	5.72	108.09	105.80
1	AA	349	A	C4-C5-C6	5.72	119.86	117.00
1	AA	655	A	C8-N9-C4	5.72	108.09	105.80
1	AA	681	A	C4-C5-C6	5.72	119.86	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1275	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1437	A	C8-N9-C4	5.72	108.09	105.80
26	BA	340	A	N3-C4-N9	5.72	131.98	127.40
26	BA	347	A	C8-N9-C4	5.72	108.09	105.80
26	BA	909	A	C4-C5-C6	5.72	119.86	117.00
26	BA	909	A	N3-C4-N9	5.72	131.98	127.40
26	BA	2198	A	C8-N9-C4	5.72	108.09	105.80
26	BA	2298	A	C8-N9-C4	5.72	108.09	105.80
26	BA	2340	A	C8-N9-C4	5.72	108.09	105.80
26	BA	2411	A	C8-N9-C4	5.72	108.09	105.80
1	AA	250	A	C8-N9-C4	5.72	108.09	105.80
1	AA	415	A	C8-N9-C4	5.72	108.09	105.80
1	AA	520	A	N3-C4-N9	5.72	131.97	127.40
1	AA	753	A	N3-C4-N9	5.72	131.98	127.40
1	AA	794	A	C8-N9-C4	5.72	108.09	105.80
1	AA	913	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1055	A	N3-C4-N9	5.72	131.98	127.40
1	AA	1080	A	N3-C4-N9	5.72	131.98	127.40
1	AA	1155	A	N3-C4-N9	5.72	131.98	127.40
1	AA	1227	A	N3-C4-N9	5.72	131.97	127.40
26	BA	861	A	N3-C4-N9	5.72	131.98	127.40
26	BA	1272	A	C8-N9-C4	5.72	108.09	105.80
26	BA	2031	A	C8-N9-C4	5.72	108.09	105.80
26	BA	2071	A	C4-C5-C6	5.72	119.86	117.00
26	BA	2082	A	C8-N9-C4	5.72	108.09	105.80
26	BA	2154	A	C4-C5-C6	5.72	119.86	117.00
26	BA	2171	A	C8-N9-C4	5.72	108.09	105.80
26	BA	2381	A	N3-C4-N9	5.72	131.97	127.40
26	BA	2886	A	C8-N9-C4	5.72	108.09	105.80
1	AA	759	A	C8-N9-C4	5.72	108.09	105.80
26	BA	149	A	C8-N9-C4	5.72	108.09	105.80
26	BA	1801	A	C8-N9-C4	5.72	108.09	105.80
26	BA	1960	A	C8-N9-C4	5.72	108.09	105.80
26	BA	2142	A	C8-N9-C4	5.72	108.09	105.80
26	BA	2270	A	C8-N9-C4	5.72	108.09	105.80
1	AA	782	A	C4-C5-N7	-5.72	107.84	110.70
1	AA	782	A	N3-C4-N9	5.72	131.97	127.40
1	AA	1368	A	N3-C4-N9	5.72	131.97	127.40
26	BA	866	A	C8-N9-C4	5.72	108.09	105.80
26	BA	1040	A	C4-C5-N7	-5.72	107.84	110.70
26	BA	1057	A	C8-N9-C4	5.72	108.09	105.80
26	BA	1304	A	N9-C4-C5	5.72	108.09	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1808	A	C8-N9-C4	5.72	108.09	105.80
26	BA	2108	A	C4-C5-N7	-5.72	107.84	110.70
1	AA	374	A	C8-N9-C4	5.71	108.09	105.80
1	AA	1000	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	1398	A	C8-N9-C4	5.71	108.09	105.80
24	AX	9	A	C8-N9-C4	5.71	108.09	105.80
26	BA	38	A	C4-C5-N7	-5.71	107.84	110.70
26	BA	156	A	N3-C4-N9	5.71	131.97	127.40
26	BA	538	A	C8-N9-C4	5.71	108.09	105.80
26	BA	734	A	C8-N9-C4	5.71	108.08	105.80
26	BA	1070	A	C8-N9-C4	5.71	108.09	105.80
26	BA	1143	A	C8-N9-C4	5.71	108.09	105.80
26	BA	2469	A	C8-N9-C4	5.71	108.09	105.80
26	BA	2542	A	N3-C4-N9	5.71	131.97	127.40
27	BB	52	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	66	A	N3-C4-N9	5.71	131.97	127.40
1	AA	649	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	695	A	C8-N9-C4	5.71	108.08	105.80
1	AA	782	A	C4-C5-C6	5.71	119.86	117.00
1	AA	825	A	N9-C4-C5	5.71	108.08	105.80
1	AA	974	A	N3-C4-N9	5.71	131.97	127.40
26	BA	621	A	C4-C5-N7	-5.71	107.84	110.70
26	BA	990	A	N3-C4-N9	5.71	131.97	127.40
26	BA	1286	A	C8-N9-C4	5.71	108.08	105.80
26	BA	2435	A	N3-C4-N9	5.71	131.97	127.40
1	AA	19	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	129	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	179	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	303	A	C8-N9-C4	5.71	108.08	105.80
1	AA	609	A	C8-N9-C4	5.71	108.08	105.80
1	AA	915	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	1213	A	C8-N9-C4	5.71	108.08	105.80
1	AA	1250	A	N3-C4-N9	5.71	131.97	127.40
23	AW	42	A	C4-C5-C6	5.71	119.86	117.00
26	BA	311	A	C8-N9-C4	5.71	108.08	105.80
26	BA	354	A	C4-C5-N7	-5.71	107.84	110.70
26	BA	1147	A	C4-C5-N7	-5.71	107.84	110.70
26	BA	1194	A	N3-C4-N9	5.71	131.97	127.40
26	BA	1509	A	N3-C4-N9	5.71	131.97	127.40
26	BA	1745	A	C8-N9-C4	5.71	108.08	105.80
26	BA	2088	A	C8-N9-C4	5.71	108.08	105.80
26	BA	2450	A	N9-C4-C5	5.71	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2513	A	N9-C4-C5	5.71	108.08	105.80
1	AA	493	A	N3-C4-N9	5.71	131.97	127.40
1	AA	908	A	C8-N9-C4	5.71	108.08	105.80
26	BA	1001	A	C4-C5-C6	5.71	119.86	117.00
26	BA	1230	A	C8-N9-C4	5.71	108.08	105.80
27	BB	29	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	412	A	C8-N9-C4	5.71	108.08	105.80
1	AA	802	A	N3-C4-N9	5.71	131.97	127.40
1	AA	1225	A	N9-C4-C5	5.71	108.08	105.80
1	AA	1256	A	C8-N9-C4	5.71	108.08	105.80
23	AW	73	A	C8-N9-C4	5.71	108.08	105.80
24	AX	41	A	C8-N9-C4	5.71	108.08	105.80
26	BA	821	A	C8-N9-C4	5.71	108.08	105.80
26	BA	1876	A	N3-C4-N9	5.71	131.97	127.40
26	BA	2170	A	C8-N9-C4	5.71	108.08	105.80
26	BA	2266	A	N3-C4-N9	5.71	131.97	127.40
1	AA	461	A	C8-N9-C4	5.71	108.08	105.80
1	AA	466	A	C8-N9-C4	5.71	108.08	105.80
1	AA	681	A	C4-C5-N7	-5.71	107.85	110.70
1	AA	1229	A	C8-N9-C4	5.71	108.08	105.80
26	BA	483	A	C8-N9-C4	5.71	108.08	105.80
26	BA	825	A	N9-C4-C5	5.71	108.08	105.80
26	BA	2019	A	C4-C5-N7	-5.71	107.85	110.70
26	BA	2135	A	N3-C4-N9	5.71	131.97	127.40
25	AY	73	A	C8-N9-C4	5.71	108.08	105.80
26	BA	89	A	N3-C4-N9	5.71	131.96	127.40
26	BA	165	A	N3-C4-N9	5.71	131.96	127.40
26	BA	1205	A	C8-N9-C4	5.71	108.08	105.80
26	BA	1347	A	C8-N9-C4	5.71	108.08	105.80
1	AA	74	A	C4-C5-C6	5.70	119.85	117.00
1	AA	327	A	C4-C5-C6	5.70	119.85	117.00
1	AA	572	A	N9-C4-C5	5.70	108.08	105.80
1	AA	1257	A	C8-N9-C4	5.70	108.08	105.80
1	AA	1492	A	N3-C4-N9	5.70	131.96	127.40
1	AA	1518	A	C8-N9-C4	5.70	108.08	105.80
25	AY	6	A	C8-N9-C4	5.70	108.08	105.80
26	BA	111	A	C4-C5-N7	-5.70	107.85	110.70
26	BA	167	A	C4-C5-C6	5.70	119.85	117.00
26	BA	480	A	N3-C4-N9	5.70	131.96	127.40
26	BA	861	A	C4-C5-N7	-5.70	107.85	110.70
26	BA	945	A	C8-N9-C4	5.70	108.08	105.80
26	BA	1111	A	C8-N9-C4	5.70	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1237	A	C4-C5-C6	5.70	119.85	117.00
26	BA	1597	A	C4-C5-N7	-5.70	107.85	110.70
26	BA	2660	A	C8-N9-C4	5.70	108.08	105.80
26	BA	2736	A	N3-C4-N9	5.70	131.96	127.40
1	AA	129	A	N9-C4-C5	5.70	108.08	105.80
1	AA	510	A	N3-C4-N9	5.70	131.96	127.40
1	AA	1158	C	C6-N1-C2	-5.70	118.02	120.30
1	AA	1250	A	C8-N9-C4	5.70	108.08	105.80
23	AW	9	A	C4-C5-C6	5.70	119.85	117.00
26	BA	127	A	N9-C4-C5	5.70	108.08	105.80
26	BA	819	A	C8-N9-C4	5.70	108.08	105.80
1	AA	160	A	C8-N9-C4	5.70	108.08	105.80
1	AA	509	A	N9-C4-C5	5.70	108.08	105.80
1	AA	900	A	C8-N9-C4	5.70	108.08	105.80
1	AA	918	A	C4-C5-N7	-5.70	107.85	110.70
1	AA	1080	A	N9-C4-C5	5.70	108.08	105.80
1	AA	1145	A	C4-C5-C6	5.70	119.85	117.00
1	AA	1216	A	C8-N9-C4	5.70	108.08	105.80
1	AA	1239	A	C4-C5-C6	5.70	119.85	117.00
1	AA	1318	A	C8-N9-C4	5.70	108.08	105.80
26	BA	265	A	C4-C5-C6	5.70	119.85	117.00
26	BA	1089	A	C8-N9-C4	5.70	108.08	105.80
26	BA	1515	A	N3-C4-N9	5.70	131.96	127.40
26	BA	1551	A	C8-N9-C4	5.70	108.08	105.80
26	BA	2268	A	C8-N9-C4	5.70	108.08	105.80
26	BA	2381	A	C4-C5-N7	-5.70	107.85	110.70
26	BA	2513	A	C4-C5-N7	-5.70	107.85	110.70
26	BA	2639	A	C4-C5-C6	5.70	119.85	117.00
26	BA	2761	A	N9-C4-C5	5.70	108.08	105.80
27	BB	104	A	C4-C5-C6	5.70	119.85	117.00
1	AA	80	A	N3-C4-N9	5.70	131.96	127.40
1	AA	109	A	C8-N9-C4	5.70	108.08	105.80
1	AA	825	A	N3-C4-N9	5.70	131.96	127.40
1	AA	1019	A	C8-N9-C4	5.70	108.08	105.80
26	BA	861	A	N9-C4-C5	5.70	108.08	105.80
26	BA	1151	A	C8-N9-C4	5.70	108.08	105.80
26	BA	1204	A	N9-C4-C5	5.70	108.08	105.80
26	BA	1403	A	C8-N9-C4	5.70	108.08	105.80
26	BA	1566	A	C8-N9-C4	5.70	108.08	105.80
26	BA	1978	A	C8-N9-C4	5.70	108.08	105.80
26	BA	2761	A	N3-C4-N9	5.70	131.96	127.40
27	BB	104	A	C8-N9-C4	5.70	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	430	A	C4-C5-C6	5.70	119.85	117.00
1	AA	498	A	N3-C4-N9	5.70	131.96	127.40
1	AA	814	A	C8-N9-C4	5.70	108.08	105.80
1	AA	1428	A	N3-C4-N9	5.70	131.96	127.40
26	BA	161	A	N3-C4-N9	5.70	131.96	127.40
26	BA	1129	A	N3-C4-N9	5.70	131.96	127.40
26	BA	2274	A	C8-N9-C4	5.70	108.08	105.80
1	AA	167	A	C8-N9-C4	5.70	108.08	105.80
26	BA	165	A	C4-C5-N7	-5.70	107.85	110.70
26	BA	504	A	C8-N9-C4	5.70	108.08	105.80
26	BA	644	A	C8-N9-C4	5.70	108.08	105.80
26	BA	1194	A	N9-C4-C5	5.70	108.08	105.80
26	BA	1916	A	C8-N9-C4	5.70	108.08	105.80
26	BA	2882	A	C8-N9-C4	5.70	108.08	105.80
1	AA	129	A	N3-C4-N9	5.69	131.96	127.40
1	AA	978	A	N3-C4-N9	5.69	131.96	127.40
26	BA	119	A	C4-C5-N7	-5.69	107.85	110.70
26	BA	226	A	C8-N9-C4	5.69	108.08	105.80
26	BA	693	A	C4-C5-N7	-5.69	107.85	110.70
26	BA	983	A	N3-C4-N9	5.69	131.96	127.40
1	AA	197	A	N3-C4-N9	5.69	131.95	127.40
1	AA	338	A	N3-C4-N9	5.69	131.95	127.40
1	AA	1163	A	C8-N9-C4	5.69	108.08	105.80
23	AW	42	A	C8-N9-C4	5.69	108.08	105.80
26	BA	207	A	C8-N9-C4	5.69	108.08	105.80
26	BA	320	A	N3-C4-N9	5.69	131.96	127.40
26	BA	354	A	C4-C5-C6	5.69	119.85	117.00
26	BA	457	A	C4-C5-N7	-5.69	107.85	110.70
26	BA	1772	A	C4-C5-C6	5.69	119.85	117.00
26	BA	2101	A	C8-N9-C4	5.69	108.08	105.80
26	BA	2451	A	C4-C5-N7	-5.69	107.85	110.70
26	BA	2632	A	N3-C4-N9	5.69	131.95	127.40
26	BA	2670	A	C8-N9-C4	5.69	108.08	105.80
1	AA	320	A	C8-N9-C4	5.69	108.08	105.80
1	AA	393	A	C4-C5-N7	-5.69	107.86	110.70
1	AA	432	A	C8-N9-C4	5.69	108.08	105.80
1	AA	1238	A	C8-N9-C4	5.69	108.08	105.80
1	AA	1350	A	C8-N9-C4	5.69	108.08	105.80
23	AW	51	A	N3-C4-N9	5.69	131.95	127.40
25	AY	14	A	C8-N9-C4	5.69	108.08	105.80
26	BA	56	A	C8-N9-C4	5.69	108.08	105.80
26	BA	218	A	C8-N9-C4	5.69	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	371	A	C4-C5-N7	-5.69	107.86	110.70
26	BA	878	A	C8-N9-C4	5.69	108.08	105.80
26	BA	2448	A	C8-N9-C4	5.69	108.08	105.80
26	BA	2482	A	C8-N9-C4	5.69	108.08	105.80
1	AA	80	A	C8-N9-C4	5.69	108.08	105.80
1	AA	282	A	C4-C5-C6	5.69	119.84	117.00
26	BA	344	A	C8-N9-C4	5.69	108.08	105.80
1	AA	174	A	C8-N9-C4	5.69	108.08	105.80
1	AA	676	A	C8-N9-C4	5.69	108.08	105.80
1	AA	753	A	C8-N9-C4	5.69	108.08	105.80
1	AA	1251	A	C8-N9-C4	5.69	108.08	105.80
26	BA	310	A	N3-C4-N9	5.69	131.95	127.40
26	BA	428	A	C8-N9-C4	5.69	108.08	105.80
26	BA	896	A	N3-C4-N9	5.69	131.95	127.40
26	BA	981	A	N3-C4-N9	5.69	131.95	127.40
26	BA	1641	A	N9-C4-C5	5.69	108.08	105.80
26	BA	1928	A	N9-C4-C5	5.69	108.08	105.80
26	BA	2101	A	C4-C5-N7	-5.69	107.86	110.70
26	BA	2176	A	N9-C4-C5	5.69	108.08	105.80
26	BA	2426	A	C8-N9-C4	5.69	108.08	105.80
26	BA	2736	A	C8-N9-C4	5.69	108.08	105.80
26	BA	2753	A	C8-N9-C4	5.69	108.08	105.80
1	AA	131	A	C4-C5-C6	5.69	119.84	117.00
1	AA	1067	A	C8-N9-C4	5.69	108.07	105.80
26	BA	144	A	C8-N9-C4	5.69	108.08	105.80
26	BA	1609	A	C8-N9-C4	5.69	108.08	105.80
26	BA	2856	A	C8-N9-C4	5.69	108.07	105.80
1	AA	143	A	C8-N9-C4	5.68	108.07	105.80
1	AA	172	A	N3-C4-N9	5.68	131.95	127.40
1	AA	210	C	C6-N1-C1'	-5.68	113.98	120.80
26	BA	270	A	C8-N9-C4	5.68	108.07	105.80
26	BA	371	A	N3-C4-N9	5.68	131.95	127.40
26	BA	470	A	C8-N9-C4	5.68	108.07	105.80
26	BA	1142	A	C4-C5-C6	5.68	119.84	117.00
26	BA	1327	A	C8-N9-C4	5.68	108.07	105.80
26	BA	1755	A	C4-C5-N7	-5.68	107.86	110.70
26	BA	2211	A	C8-N9-C4	5.68	108.07	105.80
26	BA	2418	A	C8-N9-C4	5.68	108.07	105.80
26	BA	2530	A	C8-N9-C4	5.68	108.07	105.80
26	BA	2600	A	N9-C4-C5	5.68	108.07	105.80
26	BA	2814	A	N3-C4-N9	5.68	131.95	127.40
1	AA	825	A	C4-C5-N7	-5.68	107.86	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1151	A	N9-C4-C5	5.68	108.07	105.80
26	BA	42	A	C4-C5-C6	5.68	119.84	117.00
26	BA	685	A	C8-N9-C4	5.68	108.07	105.80
26	BA	1711	A	C8-N9-C4	5.68	108.07	105.80
26	BA	1829	A	C8-N9-C4	5.68	108.07	105.80
26	BA	1952	A	C8-N9-C4	5.68	108.07	105.80
26	BA	2322	A	C4-C5-C6	5.68	119.84	117.00
26	BA	2639	A	N3-C4-N9	5.68	131.94	127.40
1	AA	819	A	C8-N9-C4	5.68	108.07	105.80
1	AA	1428	A	N9-C4-C5	5.68	108.07	105.80
25	AY	66	A	C8-N9-C4	5.68	108.07	105.80
26	BA	706	A	C8-N9-C4	5.68	108.07	105.80
26	BA	1147	A	N9-C4-C5	5.68	108.07	105.80
26	BA	1548	A	C8-N9-C4	5.68	108.07	105.80
26	BA	2448	A	N3-C4-N9	5.68	131.94	127.40
26	BA	2734	A	C8-N9-C4	5.68	108.07	105.80
1	AA	393	A	C4-C5-C6	5.68	119.84	117.00
1	AA	1236	A	C8-N9-C4	5.68	108.07	105.80
1	AA	1513	A	N3-C4-N9	5.68	131.94	127.40
22	AV	22	A	C8-N9-C4	5.68	108.07	105.80
23	AW	76	A	N3-C4-N9	5.68	131.94	127.40
26	BA	71	A	C8-N9-C4	5.68	108.07	105.80
26	BA	173	A	C8-N9-C4	5.68	108.07	105.80
26	BA	371	A	N9-C4-C5	5.68	108.07	105.80
26	BA	538	A	N3-C4-N9	5.68	131.94	127.40
26	BA	1509	A	C4-C5-C6	5.68	119.84	117.00
26	BA	1773	A	C8-N9-C4	5.68	108.07	105.80
26	BA	2749	A	C8-N9-C4	5.68	108.07	105.80
27	BB	46	A	C8-N9-C4	5.68	108.07	105.80
1	AA	139	A	C8-N9-C4	5.68	108.07	105.80
1	AA	681	A	C8-N9-C4	5.68	108.07	105.80
1	AA	1340	A	C8-N9-C4	5.68	108.07	105.80
26	BA	84	A	C4-C5-N7	-5.68	107.86	110.70
26	BA	223	A	C8-N9-C4	5.68	108.07	105.80
26	BA	265	A	N3-C4-N9	5.68	131.94	127.40
26	BA	2241	A	C4-C5-N7	-5.68	107.86	110.70
26	BA	2734	A	N3-C4-N9	5.68	131.94	127.40
1	AA	55	A	C8-N9-C4	5.68	108.07	105.80
1	AA	532	A	C8-N9-C4	5.68	108.07	105.80
1	AA	583	A	C4-C5-N7	-5.68	107.86	110.70
1	AA	704	A	C8-N9-C4	5.68	108.07	105.80
26	BA	368	A	C8-N9-C4	5.68	108.07	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	973	A	C4-C5-C6	5.68	119.84	117.00
26	BA	1244	A	C8-N9-C4	5.68	108.07	105.80
26	BA	1794	A	N3-C4-N9	5.68	131.94	127.40
26	BA	2298	A	N3-C4-N9	5.68	131.94	127.40
26	BA	2598	A	N3-C4-N9	5.68	131.94	127.40
26	BA	2657	A	C8-N9-C4	5.68	108.07	105.80
26	BA	2821	A	C8-N9-C4	5.68	108.07	105.80
1	AA	253	A	N9-C4-C5	5.67	108.07	105.80
1	AA	694	A	C8-N9-C4	5.67	108.07	105.80
1	AA	968	A	C8-N9-C4	5.67	108.07	105.80
1	AA	1413	A	C4-C5-C6	5.67	119.84	117.00
26	BA	1213	A	C8-N9-C4	5.67	108.07	105.80
26	BA	1254	A	C4-C5-C6	5.67	119.84	117.00
26	BA	1668	A	C8-N9-C4	5.67	108.07	105.80
26	BA	1746	A	C8-N9-C4	5.67	108.07	105.80
26	BA	1794	A	C4-C5-N7	-5.67	107.86	110.70
26	BA	1803	A	C4-C5-C6	5.67	119.84	117.00
26	BA	2639	A	C8-N9-C4	5.67	108.07	105.80
26	BA	2829	A	C4-C5-N7	-5.67	107.86	110.70
1	AA	572	A	N3-C4-N9	5.67	131.94	127.40
26	BA	89	A	C8-N9-C4	5.67	108.07	105.80
26	BA	299	A	N9-C4-C5	5.67	108.07	105.80
26	BA	643	A	C8-N9-C4	5.67	108.07	105.80
26	BA	1590	A	C4-C5-C6	5.67	119.84	117.00
26	BA	1735	A	C8-N9-C4	5.67	108.07	105.80
1	AA	171	A	C4-C5-N7	-5.67	107.86	110.70
1	AA	325	A	C8-N9-C4	5.67	108.07	105.80
1	AA	349	A	C8-N9-C4	5.67	108.07	105.80
1	AA	906	A	C8-N9-C4	5.67	108.07	105.80
1	AA	1055	A	C4-C5-N7	-5.67	107.86	110.70
1	AA	1287	A	C8-N9-C4	5.67	108.07	105.80
23	AW	31	A	C8-N9-C4	5.67	108.07	105.80
26	BA	21	A	C8-N9-C4	5.67	108.07	105.80
26	BA	53	A	C4-C5-C6	5.67	119.84	117.00
26	BA	345	A	C8-N9-C4	5.67	108.07	105.80
26	BA	670	A	C8-N9-C4	5.67	108.07	105.80
26	BA	742	A	N9-C4-C5	5.67	108.07	105.80
26	BA	1090	A	C8-N9-C4	5.67	108.07	105.80
26	BA	1144	A	C8-N9-C4	5.67	108.07	105.80
26	BA	1413	A	C8-N9-C4	5.67	108.07	105.80
26	BA	1772	A	C8-N9-C4	5.67	108.07	105.80
26	BA	2346	A	C8-N9-C4	5.67	108.07	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2590	A	N9-C4-C5	5.67	108.07	105.80
26	BA	2810	A	C8-N9-C4	5.67	108.07	105.80
1	AA	78	A	C8-N9-C4	5.67	108.07	105.80
1	AA	270	A	C8-N9-C4	5.67	108.07	105.80
1	AA	687	A	N3-C4-N9	5.67	131.94	127.40
1	AA	1437	A	C4-C5-C6	5.67	119.83	117.00
23	AW	42	A	C4-C5-N7	-5.67	107.86	110.70
26	BA	190	A	C8-N9-C4	5.67	108.07	105.80
26	BA	996	A	C8-N9-C4	5.67	108.07	105.80
26	BA	1347	A	N3-C4-N9	5.67	131.94	127.40
26	BA	1665	A	C8-N9-C4	5.67	108.07	105.80
26	BA	1877	A	C8-N9-C4	5.67	108.07	105.80
1	AA	196	A	C4-C5-C6	5.67	119.83	117.00
1	AA	253	A	C4-C5-N7	-5.67	107.86	110.70
1	AA	909	A	N3-C4-N9	5.67	131.94	127.40
26	BA	742	A	N3-C4-N9	5.67	131.94	127.40
26	BA	909	A	N9-C4-C5	5.67	108.07	105.80
26	BA	973	A	N3-C4-N9	5.67	131.93	127.40
26	BA	1165	A	C4-C5-N7	-5.67	107.87	110.70
26	BA	1652	A	C4-C5-N7	-5.67	107.87	110.70
26	BA	1739	A	C8-N9-C4	5.67	108.07	105.80
1	AA	533	A	N3-C4-N9	5.67	131.93	127.40
1	AA	790	A	C8-N9-C4	5.67	108.07	105.80
1	AA	802	A	C8-N9-C4	5.67	108.07	105.80
26	BA	354	A	C8-N9-C4	5.67	108.07	105.80
26	BA	454	A	N9-C4-C5	5.67	108.07	105.80
26	BA	896	A	N9-C4-C5	5.67	108.07	105.80
26	BA	918	A	N9-C4-C5	5.67	108.07	105.80
26	BA	1084	A	N9-C4-C5	5.67	108.07	105.80
26	BA	1285	A	N3-C4-N9	5.67	131.93	127.40
26	BA	1641	A	C4-C5-N7	-5.67	107.87	110.70
26	BA	1689	A	C8-N9-C4	5.67	108.07	105.80
26	BA	1780	A	C8-N9-C4	5.67	108.07	105.80
26	BA	2288	A	C8-N9-C4	5.67	108.07	105.80
1	AA	728	A	N9-C4-C5	5.67	108.07	105.80
1	AA	747	A	C8-N9-C4	5.67	108.07	105.80
1	AA	792	A	C8-N9-C4	5.67	108.07	105.80
26	BA	191	A	C8-N9-C4	5.67	108.07	105.80
26	BA	282	A	C8-N9-C4	5.67	108.07	105.80
26	BA	480	A	C4-C5-N7	-5.67	107.87	110.70
26	BA	1147	A	C4-C5-C6	5.67	119.83	117.00
26	BA	2059	A	C8-N9-C4	5.67	108.07	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2135	A	C4-C5-C6	5.67	119.83	117.00
1	AA	958	A	N9-C4-C5	5.66	108.07	105.80
1	AA	1196	A	C8-N9-C4	5.66	108.07	105.80
25	AY	58	A	C8-N9-C4	5.66	108.07	105.80
26	BA	789	A	C8-N9-C4	5.66	108.06	105.80
26	BA	988	A	N3-C4-N9	5.66	131.93	127.40
26	BA	2516	A	C8-N9-C4	5.66	108.06	105.80
26	BA	2632	A	C4-C5-N7	-5.66	107.87	110.70
27	BB	94	A	C8-N9-C4	5.66	108.07	105.80
1	AA	498	A	C8-N9-C4	5.66	108.06	105.80
1	AA	919	A	N9-C4-C5	5.66	108.06	105.80
1	AA	1246	A	C8-N9-C4	5.66	108.06	105.80
1	AA	1410	A	C4-C5-N7	-5.66	107.87	110.70
26	BA	1204	A	C4-C5-C6	5.66	119.83	117.00
26	BA	2108	A	C8-N9-C4	5.66	108.06	105.80
26	BA	2388	A	C4-C5-N7	-5.66	107.87	110.70
27	BB	58	A	N3-C4-N9	5.66	131.93	127.40
1	AA	1507	A	C8-N9-C4	5.66	108.06	105.80
26	BA	216	A	C8-N9-C4	5.66	108.06	105.80
26	BA	309	A	C8-N9-C4	5.66	108.06	105.80
26	BA	1085	A	C8-N9-C4	5.66	108.06	105.80
26	BA	1918	A	C8-N9-C4	5.66	108.06	105.80
26	BA	2147	A	C8-N9-C4	5.66	108.06	105.80
26	BA	2412	A	C8-N9-C4	5.66	108.06	105.80
26	BA	2432	A	C8-N9-C4	5.66	108.06	105.80
1	AA	60	A	C4-C5-C6	5.66	119.83	117.00
1	AA	65	A	C8-N9-C4	5.66	108.06	105.80
1	AA	1022	A	C8-N9-C4	5.66	108.06	105.80
1	AA	1092	A	N3-C4-N9	5.66	131.93	127.40
1	AA	1289	A	C8-N9-C4	5.66	108.06	105.80
26	BA	111	A	N9-C4-C5	5.66	108.06	105.80
26	BA	582	A	C8-N9-C4	5.66	108.06	105.80
26	BA	800	A	C4-C5-N7	-5.66	107.87	110.70
26	BA	911	A	C8-N9-C4	5.66	108.06	105.80
26	BA	2614	A	C8-N9-C4	5.66	108.06	105.80
26	BA	2632	A	N9-C4-C5	5.66	108.06	105.80
26	BA	2883	A	C4-C5-C6	5.66	119.83	117.00
1	AA	768	A	C8-N9-C4	5.66	108.06	105.80
1	AA	1046	A	C8-N9-C4	5.66	108.06	105.80
1	AA	1246	A	N3-C4-N9	5.66	131.93	127.40
1	AA	1499	A	C8-N9-C4	5.66	108.06	105.80
26	BA	983	A	C8-N9-C4	5.66	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	189	A	C8-N9-C4	5.66	108.06	105.80
1	AA	1333	A	N3-C4-N9	5.66	131.93	127.40
1	AA	1468	A	C8-N9-C4	5.66	108.06	105.80
23	AW	42	A	N9-C4-C5	5.66	108.06	105.80
26	BA	522	A	C8-N9-C4	5.66	108.06	105.80
26	BA	602	A	C8-N9-C4	5.66	108.06	105.80
26	BA	910	A	C8-N9-C4	5.66	108.06	105.80
26	BA	1265	A	C4-C5-C6	5.66	119.83	117.00
26	BA	1367	A	C8-N9-C4	5.66	108.06	105.80
26	BA	1590	A	C4-C5-N7	-5.66	107.87	110.70
26	BA	2829	A	C4-C5-C6	5.66	119.83	117.00
27	BB	58	A	C8-N9-C4	5.66	108.06	105.80
1	AA	533	A	C4-C5-C6	5.65	119.83	117.00
1	AA	596	A	C8-N9-C4	5.65	108.06	105.80
1	AA	1197	A	C8-N9-C4	5.65	108.06	105.80
26	BA	204	A	N9-C4-C5	5.65	108.06	105.80
26	BA	449	A	C8-N9-C4	5.65	108.06	105.80
26	BA	764	A	C4-C5-C6	5.65	119.83	117.00
26	BA	849	A	C4-C5-N7	-5.65	107.87	110.70
26	BA	1165	A	C8-N9-C4	5.65	108.06	105.80
26	BA	1359	A	N3-C4-N9	5.65	131.92	127.40
26	BA	1598	A	N3-C4-N9	5.65	131.92	127.40
1	AA	382	A	C8-N9-C4	5.65	108.06	105.80
1	AA	1130	A	C8-N9-C4	5.65	108.06	105.80
1	AA	1311	A	C8-N9-C4	5.65	108.06	105.80
25	AY	41	A	C8-N9-C4	5.65	108.06	105.80
26	BA	84	A	C4-C5-C6	5.65	119.83	117.00
26	BA	844	A	C8-N9-C4	5.65	108.06	105.80
26	BA	1237	A	N3-C4-N9	5.65	131.92	127.40
26	BA	1395	A	C8-N9-C4	5.65	108.06	105.80
26	BA	1759	A	C8-N9-C4	5.65	108.06	105.80
1	AA	3	A	N3-C4-N9	5.65	131.92	127.40
1	AA	196	A	N9-C4-C5	5.65	108.06	105.80
1	AA	288	A	C8-N9-C4	5.65	108.06	105.80
1	AA	949	A	C4-C5-N7	-5.65	107.88	110.70
23	AW	76	A	N9-C4-C5	5.65	108.06	105.80
26	BA	374	A	C8-N9-C4	5.65	108.06	105.80
26	BA	556	A	C8-N9-C4	5.65	108.06	105.80
26	BA	574	A	N9-C4-C5	5.65	108.06	105.80
26	BA	1054	A	C8-N9-C4	5.65	108.06	105.80
26	BA	1987	A	C4-C5-N7	-5.65	107.88	110.70
26	BA	2101	A	N9-C4-C5	5.65	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	199	A	C8-N9-C4	5.65	108.06	105.80
1	AA	964	A	C8-N9-C4	5.65	108.06	105.80
26	BA	2418	A	C4-C5-C6	5.65	119.82	117.00
1	AA	327	A	C8-N9-C4	5.65	108.06	105.80
1	AA	949	A	C8-N9-C4	5.65	108.06	105.80
1	AA	974	A	C8-N9-C4	5.65	108.06	105.80
22	AV	19	A	C8-N9-C4	5.65	108.06	105.80
24	AX	23	A	C8-N9-C4	5.65	108.06	105.80
24	AX	58	A	C4-C5-N7	-5.65	107.88	110.70
26	BA	38	A	C8-N9-C4	5.65	108.06	105.80
26	BA	354	A	N9-C4-C5	5.65	108.06	105.80
26	BA	447	A	C8-N9-C4	5.65	108.06	105.80
26	BA	503	A	C8-N9-C4	5.65	108.06	105.80
26	BA	1307	A	C8-N9-C4	5.65	108.06	105.80
1	AA	1410	A	N9-C4-C5	5.65	108.06	105.80
26	BA	1579	A	C8-N9-C4	5.65	108.06	105.80
1	AA	60	A	N3-C4-N9	5.64	131.92	127.40
1	AA	629	A	C8-N9-C4	5.64	108.06	105.80
1	AA	1110	A	C8-N9-C4	5.64	108.06	105.80
1	AA	1289	A	N3-C4-N9	5.64	131.91	127.40
26	BA	294	A	N3-C4-N9	5.64	131.92	127.40
26	BA	782	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1313	U	N3-C2-O2	-5.64	118.25	122.20
26	BA	2761	A	C8-N9-C4	5.64	108.06	105.80
27	BB	101	A	C8-N9-C4	5.64	108.06	105.80
27	BB	109	A	C8-N9-C4	5.64	108.06	105.80
1	AA	309	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	363	A	C8-N9-C4	5.64	108.06	105.80
1	AA	560	A	C8-N9-C4	5.64	108.06	105.80
1	AA	648	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	754	C	N3-C2-O2	-5.64	117.95	121.90
1	AA	1117	A	C8-N9-C4	5.64	108.06	105.80
1	AA	1333	A	N9-C4-C5	5.64	108.06	105.80
1	AA	1503	A	C8-N9-C4	5.64	108.06	105.80
26	BA	204	A	C4-C5-N7	-5.64	107.88	110.70
26	BA	348	A	C8-N9-C4	5.64	108.06	105.80
26	BA	478	A	C8-N9-C4	5.64	108.06	105.80
26	BA	668	A	N9-C4-C5	5.64	108.06	105.80
26	BA	936	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1014	A	C4-C5-C6	5.64	119.82	117.00
26	BA	1308	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1434	A	C8-N9-C4	5.64	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1528	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1809	A	N9-C4-C5	5.64	108.06	105.80
26	BA	1854	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1932	A	C8-N9-C4	5.64	108.06	105.80
26	BA	2478	A	N3-C4-N9	5.64	131.91	127.40
26	BA	2518	A	C8-N9-C4	5.64	108.06	105.80
26	BA	2736	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	313	A	C4-C5-N7	-5.64	107.88	110.70
23	AW	41	A	N9-C4-C5	5.64	108.06	105.80
26	BA	749	A	N3-C4-N9	5.64	131.91	127.40
26	BA	863	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1755	A	N9-C4-C5	5.64	108.06	105.80
1	AA	152	A	C8-N9-C4	5.64	108.06	105.80
1	AA	889	A	C4-C5-N7	-5.64	107.88	110.70
25	AY	21	A	C8-N9-C4	5.64	108.06	105.80
26	BA	457	A	N9-C4-C5	5.64	108.06	105.80
26	BA	1155	A	C4-C5-N7	-5.64	107.88	110.70
26	BA	1260	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1630	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1668	A	N3-C4-N9	5.64	131.91	127.40
26	BA	1701	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1805	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1821	A	N9-C4-C5	5.64	108.06	105.80
26	BA	2227	A	C8-N9-C4	5.64	108.06	105.80
26	BA	2577	A	C8-N9-C4	5.64	108.06	105.80
26	BA	2748	A	C8-N9-C4	5.64	108.06	105.80
1	AA	1042	A	N9-C4-C5	5.64	108.06	105.80
1	AA	1044	A	C8-N9-C4	5.64	108.06	105.80
1	AA	1483	A	C8-N9-C4	5.64	108.06	105.80
26	BA	538	A	C4-C5-N7	-5.64	107.88	110.70
26	BA	761	A	C8-N9-C4	5.64	108.06	105.80
26	BA	793	A	C8-N9-C4	5.64	108.06	105.80
26	BA	2288	A	C4-C5-N7	-5.64	107.88	110.70
26	BA	2388	A	N9-C4-C5	5.64	108.06	105.80
26	BA	2534	A	C8-N9-C4	5.64	108.06	105.80
1	AA	19	A	N9-C4-C5	5.64	108.05	105.80
1	AA	349	A	N3-C4-N9	5.64	131.91	127.40
1	AA	574	A	N9-C4-C5	5.64	108.06	105.80
1	AA	607	A	C8-N9-C4	5.64	108.06	105.80
1	AA	749	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	1289	A	N9-C4-C5	5.64	108.05	105.80
26	BA	38	A	N3-C4-N9	5.64	131.91	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	176	A	C8-N9-C4	5.64	108.05	105.80
26	BA	614	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1194	A	C4-C5-N7	-5.64	107.88	110.70
26	BA	1214	A	C4-C5-C6	5.64	119.82	117.00
26	BA	1336	A	C8-N9-C4	5.64	108.06	105.80
26	BA	1987	A	C8-N9-C4	5.64	108.05	105.80
26	BA	2829	A	N3-C4-N9	5.64	131.91	127.40
1	AA	182	A	N3-C4-N9	5.63	131.91	127.40
1	AA	681	A	N9-C4-C5	5.63	108.05	105.80
1	AA	694	A	N9-C4-C5	5.63	108.05	105.80
1	AA	1274	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1456	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1513	A	C8-N9-C4	5.63	108.05	105.80
26	BA	127	A	N3-C4-N9	5.63	131.91	127.40
26	BA	492	A	C8-N9-C4	5.63	108.05	105.80
26	BA	547	A	C8-N9-C4	5.63	108.05	105.80
26	BA	1214	A	C8-N9-C4	5.63	108.05	105.80
26	BA	1342	A	C8-N9-C4	5.63	108.05	105.80
26	BA	2015	A	N9-C4-C5	5.63	108.05	105.80
27	BB	39	A	C8-N9-C4	5.63	108.05	105.80
1	AA	499	A	N9-C4-C5	5.63	108.05	105.80
23	AW	51	A	C4-C5-N7	-5.63	107.88	110.70
24	AX	21	A	C8-N9-C4	5.63	108.05	105.80
26	BA	1032	A	C8-N9-C4	5.63	108.05	105.80
26	BA	1522	A	N3-C4-N9	5.63	131.91	127.40
1	AA	26	A	C8-N9-C4	5.63	108.05	105.80
1	AA	80	A	C4-C5-N7	-5.63	107.88	110.70
1	AA	356	A	C8-N9-C4	5.63	108.05	105.80
1	AA	502	A	C8-N9-C4	5.63	108.05	105.80
1	AA	784	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1176	A	C4-C5-N7	-5.63	107.88	110.70
1	AA	1311	A	N9-C4-C5	5.63	108.05	105.80
1	AA	1492	A	C8-N9-C4	5.63	108.05	105.80
26	BA	38	A	N9-C4-C5	5.63	108.05	105.80
26	BA	149	A	C4-C5-N7	-5.63	107.88	110.70
26	BA	199	A	C8-N9-C4	5.63	108.05	105.80
26	BA	300	A	N3-C4-N9	5.63	131.91	127.40
26	BA	454	A	N3-C4-N9	5.63	131.91	127.40
26	BA	529	A	N9-C4-C5	5.63	108.05	105.80
26	BA	668	A	C4-C5-C6	5.63	119.82	117.00
26	BA	905	A	C4-C5-C6	5.63	119.81	117.00
26	BA	1032	A	C4-C5-N7	-5.63	107.88	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1304	A	N3-C4-N9	5.63	131.91	127.40
26	BA	1392	A	N9-C4-C5	5.63	108.05	105.80
26	BA	1960	A	C4-C5-C6	5.63	119.81	117.00
26	BA	1981	A	C4-C5-N7	-5.63	107.88	110.70
26	BA	2154	A	N9-C4-C5	5.63	108.05	105.80
26	BA	2352	A	C8-N9-C4	5.63	108.05	105.80
26	BA	2366	A	C8-N9-C4	5.63	108.05	105.80
26	BA	2468	A	C8-N9-C4	5.63	108.05	105.80
1	AA	253	A	C8-N9-C4	5.63	108.05	105.80
1	AA	909	A	C4-C5-C6	5.63	119.81	117.00
1	AA	915	A	N3-C4-N9	5.63	131.90	127.40
26	BA	63	A	C8-N9-C4	5.63	108.05	105.80
1	AA	172	A	C4-C5-C6	5.63	119.81	117.00
1	AA	430	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1151	A	C4-C5-N7	-5.63	107.89	110.70
1	AA	1169	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1428	A	C4-C5-N7	-5.63	107.89	110.70
26	BA	44	A	C8-N9-C4	5.63	108.05	105.80
26	BA	265	A	C4-C5-N7	-5.63	107.89	110.70
26	BA	1652	A	C4-C5-C6	5.63	119.81	117.00
26	BA	2176	A	C4-C5-N7	-5.63	107.89	110.70
26	BA	2542	A	C4-C5-N7	-5.63	107.89	110.70
26	BA	2566	A	N3-C4-N9	5.63	131.90	127.40
26	BA	2600	A	C8-N9-C4	5.63	108.05	105.80
27	BB	108	A	C8-N9-C4	5.63	108.05	105.80
1	AA	195	A	C4-C5-C6	5.63	119.81	117.00
1	AA	914	A	N9-C4-C5	5.63	108.05	105.80
1	AA	1225	A	C4-C5-N7	-5.63	107.89	110.70
1	AA	1410	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1441	A	C8-N9-C4	5.63	108.05	105.80
24	AX	3	A	C8-N9-C4	5.63	108.05	105.80
26	BA	590	A	C8-N9-C4	5.63	108.05	105.80
26	BA	1794	A	N9-C4-C5	5.63	108.05	105.80
26	BA	1928	A	N3-C4-N9	5.63	131.90	127.40
26	BA	1960	A	N9-C4-C5	5.63	108.05	105.80
26	BA	2191	A	C8-N9-C4	5.63	108.05	105.80
26	BA	2278	A	C8-N9-C4	5.63	108.05	105.80
26	BA	2381	A	C8-N9-C4	5.63	108.05	105.80
26	BA	2589	A	C8-N9-C4	5.63	108.05	105.80
26	BA	2590	A	N3-C4-N9	5.63	131.90	127.40
1	AA	131	A	N3-C4-N9	5.62	131.90	127.40
1	AA	1155	A	C4-C5-N7	-5.62	107.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1480	A	C8-N9-C4	5.62	108.05	105.80
26	BA	1020	A	C8-N9-C4	5.62	108.05	105.80
26	BA	1241	A	C8-N9-C4	5.62	108.05	105.80
26	BA	1885	A	C8-N9-C4	5.62	108.05	105.80
26	BA	1981	A	N3-C4-N9	5.62	131.90	127.40
26	BA	2176	A	N3-C4-N9	5.62	131.90	127.40
1	AA	10	A	C8-N9-C4	5.62	108.05	105.80
1	AA	44	A	C8-N9-C4	5.62	108.05	105.80
1	AA	243	A	C8-N9-C4	5.62	108.05	105.80
1	AA	892	A	C8-N9-C4	5.62	108.05	105.80
1	AA	1534	A	N9-C4-C5	5.62	108.05	105.80
26	BA	207	A	N9-C4-C5	5.62	108.05	105.80
26	BA	563	A	C8-N9-C4	5.62	108.05	105.80
26	BA	1155	A	C4-C5-C6	5.62	119.81	117.00
26	BA	1427	A	N9-C4-C5	5.62	108.05	105.80
26	BA	1821	A	C4-C5-N7	-5.62	107.89	110.70
26	BA	2388	A	N3-C4-N9	5.62	131.90	127.40
26	BA	2750	A	C8-N9-C4	5.62	108.05	105.80
26	BA	2850	A	C8-N9-C4	5.62	108.05	105.80
1	AA	196	A	N3-C4-N9	5.62	131.90	127.40
1	AA	336	A	N3-C4-N9	5.62	131.90	127.40
1	AA	412	A	N3-C4-N9	5.62	131.90	127.40
1	AA	878	A	N3-C4-N9	5.62	131.90	127.40
1	AA	1204	A	C8-N9-C4	5.62	108.05	105.80
26	BA	28	A	C8-N9-C4	5.62	108.05	105.80
26	BA	155	A	C8-N9-C4	5.62	108.05	105.80
26	BA	1032	A	N9-C4-C5	5.62	108.05	105.80
26	BA	1590	A	C8-N9-C4	5.62	108.05	105.80
26	BA	1987	A	N3-C4-N9	5.62	131.90	127.40
26	BA	1987	A	N9-C4-C5	5.62	108.05	105.80
26	BA	2030	A	N9-C4-C5	5.62	108.05	105.80
26	BA	2450	A	N3-C4-N9	5.62	131.90	127.40
26	BA	2590	A	C8-N9-C4	5.62	108.05	105.80
26	BA	2600	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	263	A	N3-C4-N9	5.62	131.90	127.40
1	AA	1238	A	N9-C4-C5	5.62	108.05	105.80
26	BA	900	A	C8-N9-C4	5.62	108.05	105.80
26	BA	1039	A	C8-N9-C4	5.62	108.05	105.80
26	BA	1040	A	C4-C5-C6	5.62	119.81	117.00
26	BA	1308	A	N3-C4-N9	5.62	131.90	127.40
26	BA	1427	A	C4-C5-N7	-5.62	107.89	110.70
26	BA	1552	A	C8-N9-C4	5.62	108.05	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1853	A	N9-C4-C5	5.62	108.05	105.80
26	BA	1901	A	N9-C4-C5	5.62	108.05	105.80
26	BA	2530	A	C4-C5-N7	-5.62	107.89	110.70
27	BB	45	A	C8-N9-C4	5.62	108.05	105.80
1	AA	199	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	336	A	C8-N9-C4	5.62	108.05	105.80
1	AA	383	A	C8-N9-C4	5.62	108.05	105.80
1	AA	938	A	C8-N9-C4	5.62	108.05	105.80
1	AA	1375	A	C8-N9-C4	5.62	108.05	105.80
26	BA	749	A	C8-N9-C4	5.62	108.05	105.80
26	BA	910	A	N9-C4-C5	5.62	108.05	105.80
26	BA	1502	A	C4-C5-N7	-5.62	107.89	110.70
26	BA	1668	A	C4-C5-C6	5.62	119.81	117.00
26	BA	2097	A	C8-N9-C4	5.62	108.05	105.80
1	AA	282	A	C8-N9-C4	5.62	108.05	105.80
1	AA	320	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	918	A	N9-C4-C5	5.62	108.05	105.80
1	AA	969	A	C8-N9-C4	5.62	108.05	105.80
1	AA	1150	A	C4-C5-C6	5.62	119.81	117.00
26	BA	294	A	C4-C5-N7	-5.62	107.89	110.70
26	BA	764	A	N3-C4-N9	5.62	131.89	127.40
26	BA	1373	A	C8-N9-C4	5.62	108.05	105.80
26	BA	2247	A	N3-C4-N9	5.62	131.89	127.40
26	BA	2469	A	N9-C4-C5	5.62	108.05	105.80
1	AA	753	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	1204	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	1275	A	C8-N9-C4	5.62	108.05	105.80
1	AA	1360	A	C8-N9-C4	5.62	108.05	105.80
23	AW	66	A	C8-N9-C4	5.62	108.05	105.80
26	BA	480	A	C8-N9-C4	5.62	108.05	105.80
26	BA	722	A	C8-N9-C4	5.62	108.05	105.80
26	BA	2241	A	N9-C4-C5	5.62	108.05	105.80
26	BA	2531	A	C8-N9-C4	5.62	108.05	105.80
26	BA	2566	A	C4-C5-C6	5.62	119.81	117.00
1	AA	172	A	C8-N9-C4	5.61	108.05	105.80
1	AA	487	A	C8-N9-C4	5.61	108.05	105.80
1	AA	825	A	C8-N9-C4	5.61	108.05	105.80
26	BA	223	A	C4-C5-N7	-5.61	107.89	110.70
26	BA	1040	A	C8-N9-C4	5.61	108.05	105.80
26	BA	1226	A	N9-C4-C5	5.61	108.05	105.80
26	BA	1328	A	C8-N9-C4	5.61	108.05	105.80
26	BA	1503	A	C8-N9-C4	5.61	108.05	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1848	A	C4-C5-N7	-5.61	107.89	110.70
26	BA	1871	A	C8-N9-C4	5.61	108.05	105.80
26	BA	2406	A	C8-N9-C4	5.61	108.05	105.80
26	BA	2450	A	C4-C5-C6	5.61	119.81	117.00
26	BA	2589	A	C4-C5-C6	5.61	119.81	117.00
1	AA	482	A	C8-N9-C4	5.61	108.05	105.80
1	AA	595	A	C8-N9-C4	5.61	108.05	105.80
1	AA	1349	A	C8-N9-C4	5.61	108.05	105.80
1	AA	1413	A	N3-C4-N9	5.61	131.89	127.40
26	BA	802	A	C8-N9-C4	5.61	108.05	105.80
26	BA	941	A	C8-N9-C4	5.61	108.05	105.80
26	BA	1502	A	N9-C4-C5	5.61	108.05	105.80
26	BA	1998	A	C4-C5-N7	-5.61	107.89	110.70
26	BA	2381	A	N9-C4-C5	5.61	108.05	105.80
26	BA	2461	A	C8-N9-C4	5.61	108.05	105.80
1	AA	33	A	C8-N9-C4	5.61	108.05	105.80
1	AA	327	A	N3-C4-N9	5.61	131.89	127.40
1	AA	746	A	C8-N9-C4	5.61	108.04	105.80
1	AA	1531	A	C8-N9-C4	5.61	108.04	105.80
22	AV	20	A	C8-N9-C4	5.61	108.04	105.80
23	AW	38	A	C8-N9-C4	5.61	108.04	105.80
26	BA	101	A	C8-N9-C4	5.61	108.04	105.80
26	BA	197	A	C8-N9-C4	5.61	108.04	105.80
26	BA	460	A	C4-C5-N7	-5.61	107.89	110.70
26	BA	460	A	C8-N9-C4	5.61	108.04	105.80
26	BA	742	A	C4-C5-N7	-5.61	107.89	110.70
26	BA	1098	A	C8-N9-C4	5.61	108.04	105.80
26	BA	1156	A	C8-N9-C4	5.61	108.04	105.80
26	BA	1545	A	C8-N9-C4	5.61	108.04	105.80
26	BA	1626	A	C8-N9-C4	5.61	108.04	105.80
26	BA	1783	A	N3-C4-N9	5.61	131.89	127.40
1	AA	573	A	N9-C4-C5	5.61	108.04	105.80
1	AA	718	A	C8-N9-C4	5.61	108.04	105.80
24	AX	14	A	C8-N9-C4	5.61	108.04	105.80
26	BA	453	A	C4-C5-N7	-5.61	107.90	110.70
26	BA	454	A	C8-N9-C4	5.61	108.04	105.80
26	BA	477	A	C8-N9-C4	5.61	108.04	105.80
26	BA	2005	A	C8-N9-C4	5.61	108.04	105.80
26	BA	2868	A	N3-C4-N9	5.61	131.89	127.40
1	AA	182	A	N9-C4-C5	5.61	108.04	105.80
1	AA	313	A	C8-N9-C4	5.61	108.04	105.80
1	AA	559	A	C8-N9-C4	5.61	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1170	A	C4-C5-C6	5.61	119.80	117.00
24	AX	24	A	C8-N9-C4	5.61	108.04	105.80
26	BA	342	A	C8-N9-C4	5.61	108.04	105.80
26	BA	528	A	N3-C4-N9	5.61	131.89	127.40
26	BA	666	A	C8-N9-C4	5.61	108.04	105.80
26	BA	689	A	C8-N9-C4	5.61	108.04	105.80
26	BA	693	A	N9-C4-C5	5.61	108.04	105.80
26	BA	794	A	C8-N9-C4	5.61	108.04	105.80
26	BA	1508	A	C8-N9-C4	5.61	108.04	105.80
26	BA	1515	A	C8-N9-C4	5.61	108.04	105.80
26	BA	1809	A	C4-C5-N7	-5.61	107.90	110.70
26	BA	2406	A	C4-C5-N7	-5.61	107.90	110.70
1	AA	687	A	C4-C5-N7	-5.61	107.90	110.70
22	AV	22	A	N9-C4-C5	5.61	108.04	105.80
26	BA	149	A	N9-C4-C5	5.61	108.04	105.80
26	BA	401	A	C8-N9-C4	5.61	108.04	105.80
26	BA	574	A	C4-C5-C6	5.61	119.80	117.00
26	BA	676	A	N3-C4-N9	5.61	131.88	127.40
26	BA	1549	A	C8-N9-C4	5.61	108.04	105.80
26	BA	2009	A	C4-C5-N7	-5.61	107.90	110.70
26	BA	2868	A	N9-C4-C5	5.61	108.04	105.80
1	AA	223	A	C4-C5-N7	-5.60	107.90	110.70
26	BA	53	A	N3-C4-N9	5.60	131.88	127.40
26	BA	1610	A	N9-C4-C5	5.60	108.04	105.80
26	BA	1977	A	C8-N9-C4	5.60	108.04	105.80
26	BA	2173	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	246	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	435	A	C8-N9-C4	5.60	108.04	105.80
23	AW	41	A	C8-N9-C4	5.60	108.04	105.80
26	BA	172	A	C8-N9-C4	5.60	108.04	105.80
26	BA	195	A	C8-N9-C4	5.60	108.04	105.80
26	BA	207	A	N3-C4-N9	5.60	131.88	127.40
26	BA	503	A	C4-C5-C6	5.60	119.80	117.00
26	BA	988	A	N9-C4-C5	5.60	108.04	105.80
26	BA	2154	A	C4-C5-N7	-5.60	107.90	110.70
26	BA	2212	A	C8-N9-C4	5.60	108.04	105.80
26	BA	241	A	C4-C5-N7	-5.60	107.90	110.70
26	BA	1453	A	C8-N9-C4	5.60	108.04	105.80
26	BA	1635	A	C8-N9-C4	5.60	108.04	105.80
1	AA	179	A	N3-C4-N9	5.60	131.88	127.40
1	AA	435	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	456	A	C8-N9-C4	5.60	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	715	A	C8-N9-C4	5.60	108.04	105.80
1	AA	753	A	N9-C4-C5	5.60	108.04	105.80
1	AA	807	A	C8-N9-C4	5.60	108.04	105.80
1	AA	1151	A	C4-C5-C6	5.60	119.80	117.00
26	BA	310	A	C4-C5-N7	-5.60	107.90	110.70
26	BA	324	A	C4-C5-C6	5.60	119.80	117.00
26	BA	460	A	N9-C4-C5	5.60	108.04	105.80
26	BA	927	A	C8-N9-C4	5.60	108.04	105.80
26	BA	1054	A	C4-C5-N7	-5.60	107.90	110.70
26	BA	1165	A	N9-C4-C5	5.60	108.04	105.80
26	BA	2090	A	N3-C4-N9	5.60	131.88	127.40
26	BA	2513	A	N3-C4-N9	5.60	131.88	127.40
26	BA	2600	A	N3-C4-N9	5.60	131.88	127.40
26	BA	2758	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	26	A	N3-C4-N9	5.60	131.88	127.40
1	AA	131	A	N9-C4-C5	5.60	108.04	105.80
1	AA	236	A	N9-C4-C5	5.60	108.04	105.80
1	AA	649	A	N9-C4-C5	5.60	108.04	105.80
1	AA	913	A	N3-C4-N9	5.60	131.88	127.40
1	AA	919	A	N3-C4-N9	5.60	131.88	127.40
1	AA	1000	A	N3-C4-N9	5.60	131.88	127.40
1	AA	1093	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	1248	A	N3-C4-N9	5.60	131.88	127.40
1	AA	1431	A	C8-N9-C4	5.60	108.04	105.80
26	BA	5	A	C4-C5-N7	-5.60	107.90	110.70
26	BA	752	A	C8-N9-C4	5.60	108.04	105.80
26	BA	1009	A	N9-C4-C5	5.60	108.04	105.80
26	BA	1385	A	N9-C4-C5	5.60	108.04	105.80
26	BA	1569	A	C8-N9-C4	5.60	108.04	105.80
26	BA	1616	A	C8-N9-C4	5.60	108.04	105.80
26	BA	1960	A	C4-C5-N7	-5.60	107.90	110.70
26	BA	2094	A	C8-N9-C4	5.60	108.04	105.80
26	BA	2198	A	C4-C5-N7	-5.60	107.90	110.70
26	BA	2241	A	C8-N9-C4	5.60	108.04	105.80
26	BA	2740	A	C4-C5-N7	-5.60	107.90	110.70
22	AV	22	A	C4-C5-N7	-5.60	107.90	110.70
26	BA	152	A	C8-N9-C4	5.60	108.04	105.80
26	BA	526	A	C4-C5-N7	-5.60	107.90	110.70
26	BA	1165	A	N3-C4-N9	5.60	131.88	127.40
26	BA	2288	A	N9-C4-C5	5.60	108.04	105.80
26	BA	2837	A	C8-N9-C4	5.60	108.04	105.80
1	AA	766	A	C4-C5-N7	-5.59	107.90	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1368	A	N9-C4-C5	5.59	108.04	105.80
26	BA	825	A	C8-N9-C4	5.59	108.04	105.80
26	BA	918	A	C4-C5-N7	-5.59	107.90	110.70
26	BA	1126	A	C8-N9-C4	5.59	108.04	105.80
26	BA	1230	A	C4-C5-N7	-5.59	107.90	110.70
26	BA	1276	A	C8-N9-C4	5.59	108.04	105.80
26	BA	1553	A	C8-N9-C4	5.59	108.04	105.80
26	BA	1936	A	C8-N9-C4	5.59	108.04	105.80
26	BA	2738	A	C4-C5-N7	-5.59	107.90	110.70
26	BA	2820	A	N9-C4-C5	5.59	108.04	105.80
1	AA	243	A	N3-C4-N9	5.59	131.88	127.40
1	AA	1145	A	C8-N9-C4	5.59	108.04	105.80
26	BA	233	A	C8-N9-C4	5.59	108.04	105.80
26	BA	2225	A	C4-C5-N7	-5.59	107.90	110.70
26	BA	2298	A	C4-C5-C6	5.59	119.80	117.00
1	AA	465	A	C8-N9-C4	5.59	108.04	105.80
1	AA	640	A	C8-N9-C4	5.59	108.04	105.80
1	AA	777	A	C8-N9-C4	5.59	108.04	105.80
1	AA	780	A	N9-C4-C5	5.59	108.04	105.80
1	AA	914	A	C8-N9-C4	5.59	108.04	105.80
1	AA	1362	A	C8-N9-C4	5.59	108.04	105.80
26	BA	241	A	N3-C4-N9	5.59	131.87	127.40
26	BA	480	A	N9-C4-C5	5.59	108.04	105.80
26	BA	739	A	C8-N9-C4	5.59	108.04	105.80
26	BA	802	A	C4-C5-N7	-5.59	107.90	110.70
26	BA	861	A	C8-N9-C4	5.59	108.04	105.80
26	BA	936	A	C4-C5-N7	-5.59	107.90	110.70
26	BA	1821	A	N3-C4-N9	5.59	131.87	127.40
26	BA	2030	A	C8-N9-C4	5.59	108.04	105.80
26	BA	2434	A	N9-C4-C5	5.59	108.04	105.80
26	BA	2700	A	C8-N9-C4	5.59	108.04	105.80
26	BA	2705	A	C8-N9-C4	5.59	108.04	105.80
26	BA	2899	A	C8-N9-C4	5.59	108.04	105.80
1	AA	621	A	C8-N9-C4	5.59	108.04	105.80
1	AA	909	A	C8-N9-C4	5.59	108.04	105.80
1	AA	1105	A	C4-C5-N7	-5.59	107.91	110.70
1	AA	1229	A	C4-C5-N7	-5.59	107.91	110.70
1	AA	1269	A	N9-C4-C5	5.59	108.04	105.80
1	AA	1306	A	C8-N9-C4	5.59	108.04	105.80
1	AA	1465	A	C8-N9-C4	5.59	108.04	105.80
26	BA	155	A	C4-C5-N7	-5.59	107.91	110.70
26	BA	415	A	C8-N9-C4	5.59	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	508	A	C4-C5-N7	-5.59	107.91	110.70
26	BA	800	A	N9-C4-C5	5.59	108.04	105.80
26	BA	905	A	C8-N9-C4	5.59	108.04	105.80
26	BA	1073	A	C8-N9-C4	5.59	108.04	105.80
26	BA	1247	A	C8-N9-C4	5.59	108.03	105.80
26	BA	1284	A	C8-N9-C4	5.59	108.04	105.80
26	BA	1597	A	N9-C4-C5	5.59	108.04	105.80
26	BA	2154	A	C8-N9-C4	5.59	108.04	105.80
26	BA	2734	A	C4-C5-N7	-5.59	107.91	110.70
26	BA	2764	A	C4-C5-N7	-5.59	107.91	110.70
1	AA	802	A	C4-C5-N7	-5.59	107.91	110.70
1	AA	1492	A	C4-C5-N7	-5.59	107.91	110.70
23	AW	42	A	N3-C4-N9	5.59	131.87	127.40
26	BA	626	A	C8-N9-C4	5.59	108.03	105.80
26	BA	920	A	C8-N9-C4	5.59	108.03	105.80
26	BA	1609	A	C4-C5-N7	-5.59	107.91	110.70
26	BA	2741	A	N3-C4-N9	5.59	131.87	127.40
1	AA	77	A	C8-N9-C4	5.59	108.03	105.80
1	AA	600	A	C8-N9-C4	5.59	108.03	105.80
1	AA	681	A	N3-C4-N9	5.59	131.87	127.40
1	AA	907	A	C8-N9-C4	5.59	108.03	105.80
1	AA	1042	A	C4-C5-N7	-5.59	107.91	110.70
24	AX	26	A	C8-N9-C4	5.59	108.03	105.80
26	BA	160	A	N9-C4-C5	5.59	108.03	105.80
26	BA	182	A	C4-C5-N7	-5.59	107.91	110.70
26	BA	299	A	C4-C5-N7	-5.59	107.91	110.70
26	BA	820	A	C8-N9-C4	5.59	108.03	105.80
26	BA	917	A	C8-N9-C4	5.59	108.03	105.80
26	BA	1000	A	N9-C4-C5	5.59	108.03	105.80
26	BA	1304	A	C8-N9-C4	5.59	108.03	105.80
26	BA	1927	A	C8-N9-C4	5.59	108.03	105.80
26	BA	2019	A	C8-N9-C4	5.59	108.03	105.80
26	BA	2071	A	N3-C4-N9	5.59	131.87	127.40
26	BA	2309	A	C8-N9-C4	5.59	108.03	105.80
26	BA	2530	A	N9-C4-C5	5.59	108.03	105.80
26	BA	2565	A	N3-C4-N9	5.59	131.87	127.40
27	BB	115	A	N9-C4-C5	5.59	108.03	105.80
1	AA	411	A	N3-C4-N9	5.58	131.87	127.40
1	AA	600	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	1519	A	N9-C4-C5	5.58	108.03	105.80
26	BA	207	A	C4-C5-C6	5.58	119.79	117.00
26	BA	1502	A	C8-N9-C4	5.58	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1637	A	C8-N9-C4	5.58	108.03	105.80
26	BA	1853	A	C4-C5-N7	-5.58	107.91	110.70
26	BA	1912	A	C8-N9-C4	5.58	108.03	105.80
1	AA	782	A	C8-N9-C4	5.58	108.03	105.80
1	AA	1146	A	C4-C5-N7	-5.58	107.91	110.70
26	BA	1001	A	N3-C4-N9	5.58	131.87	127.40
26	BA	1169	A	C4-C5-N7	-5.58	107.91	110.70
26	BA	1204	A	C4-C5-N7	-5.58	107.91	110.70
26	BA	1913	A	N3-C4-N9	5.58	131.87	127.40
26	BA	2883	A	N3-C4-N9	5.58	131.87	127.40
27	BB	34	A	C4-C5-C6	5.58	119.79	117.00
1	AA	81	A	C8-N9-C4	5.58	108.03	105.80
1	AA	383	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	648	A	N9-C4-C5	5.58	108.03	105.80
1	AA	802	A	N9-C4-C5	5.58	108.03	105.80
1	AA	1111	A	C8-N9-C4	5.58	108.03	105.80
26	BA	131	A	C4-C5-N7	-5.58	107.91	110.70
26	BA	146	A	C8-N9-C4	5.58	108.03	105.80
26	BA	453	A	C8-N9-C4	5.58	108.03	105.80
26	BA	586	A	C8-N9-C4	5.58	108.03	105.80
26	BA	676	A	N9-C4-C5	5.58	108.03	105.80
26	BA	984	A	N9-C4-C5	5.58	108.03	105.80
26	BA	1048	A	C8-N9-C4	5.58	108.03	105.80
26	BA	1596	A	C8-N9-C4	5.58	108.03	105.80
26	BA	1848	A	N9-C4-C5	5.58	108.03	105.80
26	BA	1913	A	C4-C5-N7	-5.58	107.91	110.70
26	BA	1960	A	N3-C4-N9	5.58	131.87	127.40
26	BA	2406	A	N9-C4-C5	5.58	108.03	105.80
26	BA	2682	A	C8-N9-C4	5.58	108.03	105.80
26	BA	2799	A	C8-N9-C4	5.58	108.03	105.80
27	BB	115	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	253	A	N3-C4-N9	5.58	131.86	127.40
1	AA	665	A	C4-C5-N7	-5.58	107.91	110.70
26	BA	2471	A	C8-N9-C4	5.58	108.03	105.80
1	AA	309	A	N3-C4-N9	5.58	131.86	127.40
1	AA	696	A	N9-C4-C5	5.58	108.03	105.80
1	AA	915	A	N9-C4-C5	5.58	108.03	105.80
1	AA	1021	A	C8-N9-C4	5.58	108.03	105.80
1	AA	1035	A	C8-N9-C4	5.58	108.03	105.80
23	AW	21	A	C8-N9-C4	5.58	108.03	105.80
26	BA	94	A	C8-N9-C4	5.58	108.03	105.80
26	BA	899	A	C8-N9-C4	5.58	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1359	A	C4-C5-C6	5.58	119.79	117.00
26	BA	1678	A	C4-C5-N7	-5.58	107.91	110.70
26	BA	1821	A	C8-N9-C4	5.58	108.03	105.80
26	BA	2314	A	C4-C5-N7	-5.58	107.91	110.70
26	BA	2740	A	N9-C4-C5	5.58	108.03	105.80
1	AA	974	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	1092	A	N9-C4-C5	5.58	108.03	105.80
26	BA	217	A	C8-N9-C4	5.58	108.03	105.80
26	BA	423	A	C8-N9-C4	5.58	108.03	105.80
26	BA	699	A	N9-C4-C5	5.58	108.03	105.80
26	BA	2154	A	N3-C4-N9	5.58	131.86	127.40
1	AA	327	A	N9-C4-C5	5.58	108.03	105.80
1	AA	371	A	C8-N9-C4	5.58	108.03	105.80
1	AA	1246	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	1333	A	C8-N9-C4	5.58	108.03	105.80
1	AA	1410	A	N3-C4-N9	5.58	131.86	127.40
23	AW	58	A	C4-C5-N7	-5.58	107.91	110.70
24	AX	26	A	C4-C5-N7	-5.58	107.91	110.70
26	BA	84	A	N9-C4-C5	5.58	108.03	105.80
26	BA	382	A	C8-N9-C4	5.58	108.03	105.80
26	BA	877	A	C8-N9-C4	5.58	108.03	105.80
26	BA	1387	A	C8-N9-C4	5.58	108.03	105.80
26	BA	1590	A	N3-C4-N9	5.58	131.86	127.40
26	BA	1672	A	C8-N9-C4	5.58	108.03	105.80
26	BA	1755	A	N3-C4-N9	5.58	131.86	127.40
26	BA	1802	A	C8-N9-C4	5.58	108.03	105.80
26	BA	1998	A	N9-C4-C5	5.58	108.03	105.80
26	BA	2378	A	N9-C4-C5	5.58	108.03	105.80
26	BA	2721	A	C8-N9-C4	5.58	108.03	105.80
1	AA	195	A	N3-C4-N9	5.57	131.86	127.40
1	AA	602	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	909	A	N9-C4-C5	5.57	108.03	105.80
1	AA	914	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	1105	A	C8-N9-C4	5.57	108.03	105.80
1	AA	1360	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	1398	A	C4-C5-N7	-5.57	107.91	110.70
26	BA	28	A	C4-C5-N7	-5.57	107.91	110.70
26	BA	514	A	C5-C6-N1	5.57	120.49	117.70
26	BA	980	A	C8-N9-C4	5.57	108.03	105.80
26	BA	1494	A	C4-C5-N7	-5.57	107.91	110.70
26	BA	1641	A	C8-N9-C4	5.57	108.03	105.80
26	BA	2052	A	C8-N9-C4	5.57	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2736	A	N9-C4-C5	5.57	108.03	105.80
26	BA	2814	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	98	A	C8-N9-C4	5.57	108.03	105.80
1	AA	553	A	C8-N9-C4	5.57	108.03	105.80
26	BA	382	A	C4-C5-N7	-5.57	107.91	110.70
26	BA	928	A	C8-N9-C4	5.57	108.03	105.80
26	BA	2205	A	C8-N9-C4	5.57	108.03	105.80
26	BA	2476	A	C8-N9-C4	5.57	108.03	105.80
26	BA	2826	A	C8-N9-C4	5.57	108.03	105.80
1	AA	794	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	1227	A	N9-C4-C5	5.57	108.03	105.80
1	AA	1377	A	C8-N9-C4	5.57	108.03	105.80
26	BA	255	A	C8-N9-C4	5.57	108.03	105.80
26	BA	422	A	C8-N9-C4	5.57	108.03	105.80
26	BA	730	A	C8-N9-C4	5.57	108.03	105.80
26	BA	1028	A	C8-N9-C4	5.57	108.03	105.80
26	BA	1069	A	C4-C5-N7	-5.57	107.92	110.70
26	BA	1590	A	N9-C4-C5	5.57	108.03	105.80
26	BA	1749	A	C4-C5-N7	-5.57	107.92	110.70
26	BA	1872	A	N9-C4-C5	5.57	108.03	105.80
26	BA	2741	A	N9-C4-C5	5.57	108.03	105.80
26	BA	2753	A	C4-C5-N7	-5.57	107.92	110.70
26	BA	2872	A	N9-C4-C5	5.57	108.03	105.80
1	AA	223	A	C8-N9-C4	5.57	108.03	105.80
1	AA	414	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	864	A	C8-N9-C4	5.57	108.03	105.80
26	BA	959	A	C4-C5-N7	-5.57	107.92	110.70
26	BA	2009	A	C4-C5-C6	5.57	119.78	117.00
26	BA	2314	A	C8-N9-C4	5.57	108.03	105.80
1	AA	743	A	C8-N9-C4	5.57	108.03	105.80
1	AA	1437	A	N3-C4-N9	5.57	131.85	127.40
1	AA	1503	A	C4-C5-N7	-5.57	107.92	110.70
26	BA	84	A	N3-C4-N9	5.57	131.85	127.40
26	BA	161	A	N9-C4-C5	5.57	108.03	105.80
26	BA	182	A	N9-C4-C5	5.57	108.03	105.80
26	BA	352	A	C8-N9-C4	5.57	108.03	105.80
26	BA	432	A	C8-N9-C4	5.57	108.03	105.80
26	BA	1204	A	C8-N9-C4	5.57	108.03	105.80
26	BA	1477	A	C8-N9-C4	5.57	108.03	105.80
26	BA	1787	A	C8-N9-C4	5.57	108.03	105.80
26	BA	1789	A	C8-N9-C4	5.57	108.03	105.80
26	BA	1848	A	C8-N9-C4	5.57	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2564	A	N9-C4-C5	5.57	108.03	105.80
1	AA	10	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	195	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	533	A	N9-C4-C5	5.57	108.03	105.80
1	AA	622	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	759	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	1446	A	C8-N9-C4	5.57	108.03	105.80
26	BA	1050	A	C4-C5-N7	-5.57	107.92	110.70
26	BA	1204	A	N3-C4-N9	5.57	131.85	127.40
26	BA	1803	A	N3-C4-N9	5.57	131.85	127.40
26	BA	2199	A	C8-N9-C4	5.57	108.03	105.80
26	BA	2281	A	C4-C5-N7	-5.57	107.92	110.70
26	BA	2471	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	152	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	349	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	622	A	C8-N9-C4	5.56	108.03	105.80
1	AA	673	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	1519	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	1014	A	C8-N9-C4	5.56	108.03	105.80
26	BA	1783	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	2147	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	149	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	535	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	655	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	815	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	915	A	C4-C5-C6	5.56	119.78	117.00
1	AA	1093	A	N9-C4-C5	5.56	108.03	105.80
1	AA	1433	A	C8-N9-C4	5.56	108.03	105.80
23	AW	9	A	N9-C4-C5	5.56	108.03	105.80
23	AW	51	A	N9-C4-C5	5.56	108.03	105.80
26	BA	501	A	C8-N9-C4	5.56	108.03	105.80
26	BA	599	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	1069	A	N9-C4-C5	5.56	108.03	105.80
26	BA	1246	A	C8-N9-C4	5.56	108.03	105.80
26	BA	1247	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	1544	A	C8-N9-C4	5.56	108.03	105.80
26	BA	1545	A	N9-C4-C5	5.56	108.03	105.80
26	BA	2134	A	N9-C4-C5	5.56	108.03	105.80
26	BA	2247	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	2273	A	C8-N9-C4	5.56	108.03	105.80
26	BA	2738	A	N9-C4-C5	5.56	108.03	105.80
1	AA	59	A	C8-N9-C4	5.56	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	946	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	1012	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	453	A	N9-C4-C5	5.56	108.03	105.80
26	BA	2298	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	8	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	431	A	N3-C4-N9	5.56	131.85	127.40
1	AA	465	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	466	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	1012	A	C8-N9-C4	5.56	108.02	105.80
1	AA	1196	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	1288	A	C8-N9-C4	5.56	108.02	105.80
1	AA	1289	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	42	A	N3-C4-N9	5.56	131.85	127.40
26	BA	219	A	N9-C4-C5	5.56	108.02	105.80
26	BA	244	A	N9-C4-C5	5.56	108.02	105.80
26	BA	538	A	N9-C4-C5	5.56	108.02	105.80
26	BA	1089	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	1287	A	C8-N9-C4	5.56	108.02	105.80
26	BA	1307	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	1367	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	1385	A	C4-C5-C6	5.56	119.78	117.00
26	BA	1618	A	C8-N9-C4	5.56	108.02	105.80
26	BA	1668	A	N9-C4-C5	5.56	108.02	105.80
26	BA	2270	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	2741	A	C8-N9-C4	5.56	108.02	105.80
26	BA	2776	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	344	A	C8-N9-C4	5.56	108.02	105.80
1	AA	642	A	N9-C4-C5	5.56	108.02	105.80
1	AA	712	A	C8-N9-C4	5.56	108.02	105.80
1	AA	919	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	1170	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	262	A	N9-C4-C5	5.56	108.02	105.80
26	BA	631	A	C8-N9-C4	5.56	108.02	105.80
26	BA	792	A	C8-N9-C4	5.56	108.02	105.80
26	BA	829	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	1268	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	1268	A	C8-N9-C4	5.56	108.02	105.80
26	BA	1586	A	C8-N9-C4	5.56	108.02	105.80
26	BA	2425	A	C8-N9-C4	5.56	108.02	105.80
26	BA	2634	A	C4-C5-N7	-5.56	107.92	110.70
27	BB	58	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	608	A	C8-N9-C4	5.56	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	831	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	330	A	C8-N9-C4	5.56	108.02	105.80
26	BA	718	A	C4-C5-N7	-5.56	107.92	110.70
26	BA	739	A	N9-C4-C5	5.56	108.02	105.80
26	BA	1010	A	N9-C4-C5	5.56	108.02	105.80
1	AA	7	A	C8-N9-C4	5.55	108.02	105.80
1	AA	139	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	306	A	C8-N9-C4	5.55	108.02	105.80
1	AA	363	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	533	A	C8-N9-C4	5.55	108.02	105.80
1	AA	553	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	649	A	C8-N9-C4	5.55	108.02	105.80
26	BA	231	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	422	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	508	A	C8-N9-C4	5.55	108.02	105.80
26	BA	526	A	N9-C4-C5	5.55	108.02	105.80
26	BA	1247	A	N9-C4-C5	5.55	108.02	105.80
26	BA	1286	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	1593	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	2435	A	N9-C4-C5	5.55	108.02	105.80
1	AA	167	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	236	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	1019	A	C4-C5-N7	-5.55	107.92	110.70
22	AV	17	A	C8-N9-C4	5.55	108.02	105.80
26	BA	833	A	N9-C4-C5	5.55	108.02	105.80
26	BA	849	A	N9-C4-C5	5.55	108.02	105.80
26	BA	1272	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	1342	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	1515	A	N9-C4-C5	5.55	108.02	105.80
26	BA	1668	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	2369	A	C8-N9-C4	5.55	108.02	105.80
26	BA	2868	A	C4-C5-C6	5.55	119.78	117.00
1	AA	152	A	N9-C4-C5	5.55	108.02	105.80
1	AA	182	A	C4-C5-C6	5.55	119.78	117.00
1	AA	712	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	878	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	42	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	191	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	322	A	C8-N9-C4	5.55	108.02	105.80
26	BA	1803	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	1952	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	2879	A	C8-N9-C4	5.55	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2882	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	2887	A	C8-N9-C4	5.55	108.02	105.80
1	AA	171	A	C8-N9-C4	5.55	108.02	105.80
1	AA	573	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	663	A	N9-C4-C5	5.55	108.02	105.80
1	AA	702	A	C8-N9-C4	5.55	108.02	105.80
1	AA	958	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	1246	A	N9-C4-C5	5.55	108.02	105.80
1	AA	1287	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	1346	A	C8-N9-C4	5.55	108.02	105.80
26	BA	95	A	C8-N9-C4	5.55	108.02	105.80
26	BA	156	A	C8-N9-C4	5.55	108.02	105.80
26	BA	699	A	C4-C5-N7	-5.55	107.92	110.70
26	BA	1175	A	C8-N9-C4	5.55	108.02	105.80
26	BA	1274	A	N9-C4-C5	5.55	108.02	105.80
26	BA	1772	A	N3-C4-N9	5.55	131.84	127.40
26	BA	1803	A	C8-N9-C4	5.55	108.02	105.80
26	BA	1853	A	C8-N9-C4	5.55	108.02	105.80
26	BA	2058	A	N9-C4-C5	5.55	108.02	105.80
1	AA	389	A	C8-N9-C4	5.55	108.02	105.80
26	BA	693	A	C8-N9-C4	5.55	108.02	105.80
26	BA	1032	A	N3-C4-N9	5.55	131.84	127.40
26	BA	1095	A	C4-C5-N7	-5.55	107.93	110.70
26	BA	1095	A	C8-N9-C4	5.55	108.02	105.80
26	BA	1237	A	C4-C5-N7	-5.55	107.93	110.70
26	BA	1913	A	N9-C4-C5	5.55	108.02	105.80
26	BA	2829	A	N9-C4-C5	5.55	108.02	105.80
26	BA	2850	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	72	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	238	A	C8-N9-C4	5.55	108.02	105.80
1	AA	309	A	C8-N9-C4	5.55	108.02	105.80
1	AA	373	A	C8-N9-C4	5.55	108.02	105.80
1	AA	696	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	845	A	C8-N9-C4	5.55	108.02	105.80
1	AA	1252	A	N9-C4-C5	5.55	108.02	105.80
1	AA	1332	A	N9-C4-C5	5.55	108.02	105.80
26	BA	422	A	N9-C4-C5	5.55	108.02	105.80
26	BA	471	A	C8-N9-C4	5.55	108.02	105.80
26	BA	668	A	C8-N9-C4	5.55	108.02	105.80
26	BA	743	A	C8-N9-C4	5.55	108.02	105.80
26	BA	975	A	C8-N9-C4	5.55	108.02	105.80
26	BA	1001	A	N9-C4-C5	5.55	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1630	A	C4-C5-C6	5.55	119.77	117.00
26	BA	1786	A	C4-C5-N7	-5.55	107.93	110.70
26	BA	1899	A	N9-C4-C5	5.55	108.02	105.80
26	BA	71	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	472	A	N9-C4-C5	5.54	108.02	105.80
26	BA	529	A	N3-C4-N9	5.54	131.84	127.40
26	BA	621	A	N3-C4-N9	5.54	131.84	127.40
26	BA	996	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	1700	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	1773	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	1953	A	N9-C4-C5	5.54	108.02	105.80
26	BA	2813	A	N9-C4-C5	5.54	108.02	105.80
1	AA	80	A	N9-C4-C5	5.54	108.02	105.80
1	AA	223	A	N9-C4-C5	5.54	108.02	105.80
1	AA	1146	A	C8-N9-C4	5.54	108.02	105.80
1	AA	1349	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	216	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	1000	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	1127	A	N9-C4-C5	5.54	108.02	105.80
26	BA	2060	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	2090	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	2478	A	C4-C5-C6	5.54	119.77	117.00
1	AA	51	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	452	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	600	A	N9-C4-C5	5.54	108.02	105.80
1	AA	1170	A	C8-N9-C4	5.54	108.02	105.80
1	AA	1428	A	C8-N9-C4	5.54	108.02	105.80
26	BA	89	A	N9-C4-C5	5.54	108.02	105.80
26	BA	155	A	N9-C4-C5	5.54	108.02	105.80
26	BA	160	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	223	A	N9-C4-C5	5.54	108.02	105.80
26	BA	1009	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	1503	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	1503	A	N9-C4-C5	5.54	108.02	105.80
26	BA	1928	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	2433	A	C8-N9-C4	5.54	108.02	105.80
26	BA	2792	A	C8-N9-C4	5.54	108.02	105.80
27	BB	115	A	C8-N9-C4	5.54	108.02	105.80
1	AA	78	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	366	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	2080	A	C8-N9-C4	5.54	108.02	105.80
26	BA	2873	A	C4-C5-N7	-5.54	107.93	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	3	A	N9-C4-C5	5.54	108.02	105.80
1	AA	313	A	N9-C4-C5	5.54	108.02	105.80
1	AA	383	A	N9-C4-C5	5.54	108.02	105.80
1	AA	456	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	1238	A	C4-C5-C6	5.54	119.77	117.00
26	BA	101	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	541	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	592	A	C8-N9-C4	5.54	108.02	105.80
26	BA	739	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	1246	A	N9-C4-C5	5.54	108.02	105.80
26	BA	1610	A	C8-N9-C4	5.54	108.02	105.80
26	BA	2134	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	2750	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	2814	A	C8-N9-C4	5.54	108.02	105.80
1	AA	130	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	461	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	510	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	1197	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	1001	A	C8-N9-C4	5.54	108.02	105.80
26	BA	2298	A	N9-C4-C5	5.54	108.02	105.80
26	BA	2314	A	N9-C4-C5	5.54	108.02	105.80
26	BA	2377	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	65	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	574	A	N3-C4-N9	5.54	131.83	127.40
1	AA	860	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	1105	A	N9-C4-C5	5.54	108.01	105.80
1	AA	1204	A	N9-C4-C5	5.54	108.01	105.80
1	AA	1476	A	C8-N9-C4	5.54	108.01	105.80
26	BA	501	A	N9-C4-C5	5.54	108.01	105.80
26	BA	529	A	C4-C5-C6	5.54	119.77	117.00
26	BA	621	A	C4-C5-C6	5.54	119.77	117.00
26	BA	804	A	C8-N9-C4	5.54	108.01	105.80
26	BA	1307	A	N9-C4-C5	5.54	108.01	105.80
26	BA	1916	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	2003	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	2030	A	C4-C5-N7	-5.54	107.93	110.70
26	BA	2459	A	C8-N9-C4	5.54	108.02	105.80
26	BA	2632	A	C8-N9-C4	5.54	108.01	105.80
26	BA	2873	A	N9-C4-C5	5.54	108.01	105.80
27	BB	53	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	66	A	C4-C5-N7	-5.53	107.93	110.70
1	AA	695	A	C4-C5-N7	-5.53	107.93	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	919	A	C8-N9-C4	5.53	108.01	105.80
1	AA	1016	A	N9-C4-C5	5.53	108.01	105.80
1	AA	1408	A	C4-C5-N7	-5.53	107.93	110.70
26	BA	195	A	C4-C5-N7	-5.53	107.93	110.70
26	BA	270	A	C4-C5-N7	-5.53	107.93	110.70
26	BA	344	A	C4-C5-N7	-5.53	107.93	110.70
26	BA	501	A	C4-C5-N7	-5.53	107.93	110.70
26	BA	574	A	C4-C5-N7	-5.53	107.93	110.70
26	BA	1505	A	C8-N9-C4	5.53	108.01	105.80
26	BA	1522	A	C4-C5-C6	5.53	119.77	117.00
26	BA	2327	A	N9-C4-C5	5.53	108.01	105.80
26	BA	2734	A	N9-C4-C5	5.53	108.01	105.80
26	BA	2821	A	C4-C5-N7	-5.53	107.93	110.70
1	AA	53	A	C4-C5-N7	-5.53	107.93	110.70
26	BA	529	A	C8-N9-C4	5.53	108.01	105.80
26	BA	2183	A	C8-N9-C4	5.53	108.01	105.80
26	BA	2566	A	C4-C5-N7	-5.53	107.93	110.70
26	BA	2899	A	C4-C5-N7	-5.53	107.93	110.70
1	AA	139	A	N9-C4-C5	5.53	108.01	105.80
1	AA	892	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	1171	A	C8-N9-C4	5.53	108.01	105.80
1	AA	1191	A	C8-N9-C4	5.53	108.01	105.80
1	AA	1413	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	1531	A	C4-C5-N7	-5.53	107.94	110.70
26	BA	959	A	C8-N9-C4	5.53	108.01	105.80
26	BA	1142	A	N3-C4-N9	5.53	131.82	127.40
26	BA	1744	A	C8-N9-C4	5.53	108.01	105.80
26	BA	2009	A	N3-C4-N9	5.53	131.82	127.40
26	BA	2042	A	C8-N9-C4	5.53	108.01	105.80
26	BA	2183	A	C4-C5-N7	-5.53	107.93	110.70
26	BA	2435	A	C4-C5-N7	-5.53	107.93	110.70
26	BA	2547	A	C8-N9-C4	5.53	108.01	105.80
26	BA	2711	A	N9-C4-C5	5.53	108.01	105.80
1	AA	130	A	C8-N9-C4	5.53	108.01	105.80
1	AA	143	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	533	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	1513	A	C4-C5-N7	-5.53	107.94	110.70
26	BA	156	A	N9-C4-C5	5.53	108.01	105.80
26	BA	1189	A	C4-C5-N7	-5.53	107.94	110.70
26	BA	2587	A	C8-N9-C4	5.53	108.01	105.80
1	AA	155	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	162	A	C8-N9-C4	5.53	108.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	320	A	N9-C4-C5	5.53	108.01	105.80
1	AA	579	A	C8-N9-C4	5.53	108.01	105.80
1	AA	665	A	C4-C5-C6	5.53	119.76	117.00
1	AA	1055	A	N9-C4-C5	5.53	108.01	105.80
1	AA	1176	A	C8-N9-C4	5.53	108.01	105.80
1	AA	1324	A	C8-N9-C4	5.53	108.01	105.80
1	AA	1441	A	C4-C5-N7	-5.53	107.94	110.70
23	AW	26	A	C4-C5-N7	-5.53	107.94	110.70
23	AW	58	A	N9-C4-C5	5.53	108.01	105.80
26	BA	14	A	C8-N9-C4	5.53	108.01	105.80
26	BA	49	A	C4-C5-N7	-5.53	107.94	110.70
26	BA	265	A	N9-C4-C5	5.53	108.01	105.80
26	BA	477	A	C4-C5-N7	-5.53	107.94	110.70
26	BA	1393	A	N9-C4-C5	5.53	108.01	105.80
26	BA	1847	A	C4-C5-N7	-5.53	107.94	110.70
26	BA	2376	A	C8-N9-C4	5.53	108.01	105.80
1	AA	44	A	N3-C4-N9	5.53	131.82	127.40
1	AA	460	A	C8-N9-C4	5.53	108.01	105.80
1	AA	712	A	N9-C4-C5	5.53	108.01	105.80
1	AA	1360	A	N9-C4-C5	5.53	108.01	105.80
1	AA	1418	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	1492	A	N9-C4-C5	5.53	108.01	105.80
24	AX	41	A	C4-C5-N7	-5.53	107.94	110.70
26	BA	181	A	C8-N9-C4	5.53	108.01	105.80
26	BA	348	A	C4-C5-N7	-5.53	107.94	110.70
26	BA	502	A	C8-N9-C4	5.53	108.01	105.80
26	BA	515	A	C8-N9-C4	5.53	108.01	105.80
26	BA	735	A	N9-C4-C5	5.53	108.01	105.80
26	BA	1268	A	N9-C4-C5	5.53	108.01	105.80
26	BA	1679	A	C8-N9-C4	5.53	108.01	105.80
26	BA	1717	A	C4-C5-N7	-5.53	107.94	110.70
26	BA	1937	A	C8-N9-C4	5.53	108.01	105.80
26	BA	2899	A	N9-C4-C5	5.53	108.01	105.80
26	BA	428	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	466	A	N3-C4-N9	5.52	131.82	127.40
26	BA	1508	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	493	A	C8-N9-C4	5.52	108.01	105.80
1	AA	1117	A	C4-C5-N7	-5.52	107.94	110.70
24	AX	26	A	N9-C4-C5	5.52	108.01	105.80
26	BA	6	A	N9-C4-C5	5.52	108.01	105.80
26	BA	371	A	C4-C5-C6	5.52	119.76	117.00
26	BA	802	A	N9-C4-C5	5.52	108.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	959	A	N9-C4-C5	5.52	108.01	105.80
26	BA	988	A	C8-N9-C4	5.52	108.01	105.80
26	BA	1384	A	C8-N9-C4	5.52	108.01	105.80
26	BA	2108	A	N3-C4-N9	5.52	131.82	127.40
26	BA	2577	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	2598	A	N9-C4-C5	5.52	108.01	105.80
26	BA	2726	A	C4-C5-N7	-5.52	107.94	110.70
27	BB	101	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	298	A	C8-N9-C4	5.52	108.01	105.80
1	AA	371	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	613	A	C8-N9-C4	5.52	108.01	105.80
26	BA	2268	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	26	A	N9-C4-C5	5.52	108.01	105.80
1	AA	66	A	N9-C4-C5	5.52	108.01	105.80
1	AA	860	A	C8-N9-C4	5.52	108.01	105.80
1	AA	969	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	1155	A	N9-C4-C5	5.52	108.01	105.80
1	AA	1271	A	C8-N9-C4	5.52	108.01	105.80
1	AA	1363	A	C8-N9-C4	5.52	108.01	105.80
24	AX	9	A	C4-C5-N7	-5.52	107.94	110.70
25	AY	23	A	C8-N9-C4	5.52	108.01	105.80
26	BA	6	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	172	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	219	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	244	A	C8-N9-C4	5.52	108.01	105.80
26	BA	466	A	N9-C4-C5	5.52	108.01	105.80
26	BA	655	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	788	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	988	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	1175	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	1254	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	1286	A	N9-C4-C5	5.52	108.01	105.80
26	BA	1287	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	1746	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	2009	A	N9-C4-C5	5.52	108.01	105.80
26	BA	2071	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	2733	A	C8-N9-C4	5.52	108.01	105.80
26	BA	2741	A	C4-C5-C6	5.52	119.76	117.00
27	BB	53	A	C8-N9-C4	5.52	108.01	105.80
1	AA	630	A	C8-N9-C4	5.52	108.01	105.80
1	AA	1227	A	C4-C5-N7	-5.52	107.94	110.70
24	AX	14	A	C4-C5-N7	-5.52	107.94	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	131	A	C8-N9-C4	5.52	108.01	105.80
26	BA	309	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	804	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	943	A	C8-N9-C4	5.52	108.01	105.80
26	BA	1069	A	C8-N9-C4	5.52	108.01	105.80
26	BA	1098	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	1103	A	C8-N9-C4	5.52	108.01	105.80
26	BA	1246	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	1427	A	N3-C4-N9	5.52	131.81	127.40
26	BA	1610	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	1847	A	C8-N9-C4	5.52	108.01	105.80
26	BA	2170	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	2753	A	N9-C4-C5	5.52	108.01	105.80
27	BB	119	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	205	A	C8-N9-C4	5.52	108.01	105.80
1	AA	1480	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	118	A	N9-C4-C5	5.52	108.01	105.80
26	BA	1067	A	C8-N9-C4	5.52	108.01	105.80
26	BA	1392	A	C4-C5-N7	-5.52	107.94	110.70
26	BA	1618	A	N9-C4-C5	5.52	108.01	105.80
26	BA	2173	A	N9-C4-C5	5.52	108.01	105.80
1	AA	161	A	C8-N9-C4	5.51	108.01	105.80
1	AA	228	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	288	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	655	A	N9-C4-C5	5.51	108.01	105.80
1	AA	845	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	1437	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	19	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	217	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	300	A	N9-C4-C5	5.51	108.00	105.80
26	BA	632	A	N9-C4-C5	5.51	108.01	105.80
26	BA	1285	A	N9-C4-C5	5.51	108.01	105.80
26	BA	1871	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	2077	A	C8-N9-C4	5.51	108.01	105.80
26	BA	2411	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	2577	A	N9-C4-C5	5.51	108.01	105.80
26	BA	2657	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	7	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	1513	A	N9-C4-C5	5.51	108.00	105.80
23	AW	38	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	144	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	320	A	C4-C5-N7	-5.51	107.94	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	508	A	N9-C4-C5	5.51	108.00	105.80
26	BA	911	A	N9-C4-C5	5.51	108.00	105.80
26	BA	1129	A	N9-C4-C5	5.51	108.00	105.80
26	BA	1133	A	C8-N9-C4	5.51	108.00	105.80
26	BA	1347	A	N9-C4-C5	5.51	108.00	105.80
26	BA	1353	A	C8-N9-C4	5.51	108.00	105.80
26	BA	1571	A	C8-N9-C4	5.51	108.00	105.80
26	BA	2015	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	59	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	583	A	N9-C4-C5	5.51	108.00	105.80
1	AA	1176	A	N9-C4-C5	5.51	108.00	105.80
1	AA	1377	A	C4-C5-N7	-5.51	107.94	110.70
25	AY	69	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	471	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	599	A	C8-N9-C4	5.51	108.00	105.80
26	BA	668	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	899	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	927	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	1095	A	N9-C4-C5	5.51	108.00	105.80
26	BA	1342	A	N9-C4-C5	5.51	108.00	105.80
26	BA	1544	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	1698	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	2448	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	2453	A	C8-N9-C4	5.51	108.00	105.80
1	AA	151	A	C4-C5-C6	5.51	119.75	117.00
1	AA	228	A	C8-N9-C4	5.51	108.00	105.80
1	AA	327	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	572	A	C4-C5-N7	-5.51	107.95	110.70
1	AA	974	A	N9-C4-C5	5.51	108.00	105.80
1	AA	1180	A	C8-N9-C4	5.51	108.00	105.80
1	AA	1280	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	347	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	627	A	C8-N9-C4	5.51	108.00	105.80
26	BA	749	A	N9-C4-C5	5.51	108.00	105.80
26	BA	788	A	N9-C4-C5	5.51	108.00	105.80
26	BA	1084	A	C4-C5-N7	-5.51	107.94	110.70
26	BA	1598	A	N9-C4-C5	5.51	108.00	105.80
26	BA	1689	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	2082	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	2225	A	N3-C4-N9	5.51	131.81	127.40
26	BA	2513	A	C8-N9-C4	5.51	108.00	105.80
26	BA	2534	A	C4-C5-N7	-5.51	107.94	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BB	78	A	N3-C4-N9	5.51	131.81	127.40
1	AA	149	A	N9-C4-C5	5.51	108.00	105.80
26	BA	181	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	918	A	C8-N9-C4	5.51	108.00	105.80
26	BA	1127	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	2503	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	2900	A	C4-C5-N7	-5.51	107.95	110.70
1	AA	155	A	C8-N9-C4	5.51	108.00	105.80
1	AA	687	A	N9-C4-C5	5.51	108.00	105.80
1	AA	878	A	N9-C4-C5	5.51	108.00	105.80
1	AA	900	A	C4-C5-N7	-5.51	107.95	110.70
1	AA	978	A	C4-C5-N7	-5.51	107.95	110.70
1	AA	1014	A	N9-C4-C5	5.51	108.00	105.80
23	AW	14	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	262	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	945	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	1057	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	1205	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	1545	A	N3-C4-N9	5.51	131.81	127.40
26	BA	1618	A	C4-C5-N7	-5.51	107.95	110.70
26	BA	64	A	C8-N9-C4	5.50	108.00	105.80
26	BA	572	A	C8-N9-C4	5.50	108.00	105.80
26	BA	602	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	1302	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	2478	A	N9-C4-C5	5.50	108.00	105.80
1	AA	181	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	374	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	1036	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	1229	A	N9-C4-C5	5.50	108.00	105.80
26	BA	231	A	C8-N9-C4	5.50	108.00	105.80
26	BA	262	A	C8-N9-C4	5.50	108.00	105.80
26	BA	721	A	N9-C4-C5	5.50	108.00	105.80
26	BA	804	A	N9-C4-C5	5.50	108.00	105.80
26	BA	1347	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	1366	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	1889	A	C8-N9-C4	5.50	108.00	105.80
26	BA	2727	A	C8-N9-C4	5.50	108.00	105.80
1	AA	274	A	C8-N9-C4	5.50	108.00	105.80
1	AA	364	A	C8-N9-C4	5.50	108.00	105.80
1	AA	949	A	N9-C4-C5	5.50	108.00	105.80
1	AA	1092	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	1111	A	C4-C5-N7	-5.50	107.95	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1319	A	C8-N9-C4	5.50	108.00	105.80
1	AA	1441	A	N9-C4-C5	5.50	108.00	105.80
23	AW	26	A	C8-N9-C4	5.50	108.00	105.80
26	BA	213	A	C8-N9-C4	5.50	108.00	105.80
26	BA	241	A	C4-C5-C6	5.50	119.75	117.00
26	BA	244	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	345	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	346	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	783	A	N3-C4-N9	5.50	131.80	127.40
26	BA	936	A	N9-C4-C5	5.50	108.00	105.80
26	BA	1552	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	1652	A	N3-C4-N9	5.50	131.80	127.40
26	BA	1970	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	2090	A	N9-C4-C5	5.50	108.00	105.80
26	BA	2322	A	N3-C4-N9	5.50	131.80	127.40
26	BA	2564	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	648	A	C8-N9-C4	5.50	108.00	105.80
26	BA	515	A	N9-C4-C5	5.50	108.00	105.80
26	BA	2135	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	2309	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	456	A	N9-C4-C5	5.50	108.00	105.80
1	AA	663	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	1261	A	C8-N9-C4	5.50	108.00	105.80
1	AA	1531	A	N9-C4-C5	5.50	108.00	105.80
26	BA	241	A	N9-C4-C5	5.50	108.00	105.80
26	BA	332	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	502	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	1169	A	C8-N9-C4	5.50	108.00	105.80
26	BA	1354	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	1496	A	C8-N9-C4	5.50	108.00	105.80
26	BA	1515	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	1757	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	1791	A	N9-C4-C5	5.50	108.00	105.80
26	BA	2266	A	N9-C4-C5	5.50	108.00	105.80
1	AA	642	A	C8-N9-C4	5.50	108.00	105.80
1	AA	913	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	1036	A	N9-C4-C5	5.50	108.00	105.80
23	AW	9	A	C4-C5-N7	-5.50	107.95	110.70
23	AW	76	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	89	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	199	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	203	A	C8-N9-C4	5.50	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	753	A	N9-C4-C5	5.50	108.00	105.80
26	BA	1214	A	N9-C4-C5	5.50	108.00	105.80
26	BA	1551	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	2352	A	C4-C5-N7	-5.50	107.95	110.70
26	BA	2453	A	N9-C4-C5	5.50	108.00	105.80
26	BA	2634	A	N9-C4-C5	5.50	108.00	105.80
27	BB	94	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	448	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	642	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	1012	A	N9-C4-C5	5.50	108.00	105.80
1	AA	1413	A	N9-C4-C5	5.50	108.00	105.80
26	BA	126	A	C8-N9-C4	5.50	108.00	105.80
26	BA	742	A	C8-N9-C4	5.50	108.00	105.80
26	BA	909	A	C8-N9-C4	5.50	108.00	105.80
26	BA	2850	A	N9-C4-C5	5.50	108.00	105.80
1	AA	55	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	673	A	N9-C4-C5	5.49	108.00	105.80
1	AA	1251	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	125	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	156	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	608	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	661	A	C8-N9-C4	5.49	108.00	105.80
26	BA	783	A	C4-C5-C6	5.49	119.75	117.00
26	BA	1142	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	1762	A	N9-C4-C5	5.49	108.00	105.80
26	BA	2634	A	C8-N9-C4	5.49	108.00	105.80
26	BA	2851	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	60	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	325	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	553	A	N9-C4-C5	5.49	108.00	105.80
1	AA	749	A	N9-C4-C5	5.49	108.00	105.80
23	AW	59	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	126	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	352	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	1098	A	N9-C4-C5	5.49	108.00	105.80
26	BA	2147	A	N9-C4-C5	5.49	108.00	105.80
26	BA	2516	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	78	A	N9-C4-C5	5.49	108.00	105.80
1	AA	119	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	130	A	N9-C4-C5	5.49	108.00	105.80
1	AA	729	A	C8-N9-C4	5.49	108.00	105.80
23	AW	21	A	C4-C5-N7	-5.49	107.95	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	382	A	N9-C4-C5	5.49	108.00	105.80
26	BA	781	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	1274	A	C8-N9-C4	5.49	108.00	105.80
26	BA	1610	A	N3-C4-N9	5.49	131.79	127.40
26	BA	1927	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	2198	A	N9-C4-C5	5.49	108.00	105.80
26	BA	2266	A	C8-N9-C4	5.49	108.00	105.80
26	BA	2435	A	C8-N9-C4	5.49	108.00	105.80
26	BA	2711	A	C4-C5-N7	-5.49	107.95	110.70
26	BA	2764	A	C8-N9-C4	5.49	108.00	105.80
26	BA	2814	A	N9-C4-C5	5.49	108.00	105.80
1	AA	716	A	C8-N9-C4	5.49	108.00	105.80
1	AA	937	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	1179	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	1196	A	N9-C4-C5	5.49	108.00	105.80
1	AA	1519	A	C8-N9-C4	5.49	108.00	105.80
23	AW	59	A	C8-N9-C4	5.49	108.00	105.80
26	BA	514	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	563	A	N9-C4-C5	5.49	108.00	105.80
26	BA	592	A	N9-C4-C5	5.49	108.00	105.80
26	BA	727	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	751	A	C8-N9-C4	5.49	108.00	105.80
26	BA	975	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	1000	A	C8-N9-C4	5.49	108.00	105.80
26	BA	1419	A	N3-C4-N9	5.49	131.79	127.40
26	BA	1889	A	N9-C4-C5	5.49	108.00	105.80
26	BA	2031	A	N9-C4-C5	5.49	108.00	105.80
26	BA	2126	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	2565	A	N9-C4-C5	5.49	108.00	105.80
1	AA	71	A	C8-N9-C4	5.49	108.00	105.80
1	AA	120	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	349	A	N9-C4-C5	5.49	108.00	105.80
1	AA	435	A	N9-C4-C5	5.49	108.00	105.80
1	AA	1275	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	131	A	N9-C4-C5	5.49	108.00	105.80
26	BA	217	A	N9-C4-C5	5.49	108.00	105.80
26	BA	374	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	909	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	1632	A	C8-N9-C4	5.49	108.00	105.80
26	BA	1640	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	1877	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	262	A	C8-N9-C4	5.49	107.99	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	393	A	C8-N9-C4	5.49	108.00	105.80
1	AA	635	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	906	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	1004	A	C8-N9-C4	5.49	107.99	105.80
1	AA	1145	A	N9-C4-C5	5.49	107.99	105.80
1	AA	1493	A	N3-C4-N9	5.49	131.79	127.40
26	BA	482	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	592	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	734	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	1111	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	1143	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	1508	A	N9-C4-C5	5.49	108.00	105.80
26	BA	1586	A	C4-C5-N7	-5.49	107.96	110.70
26	BA	2225	A	C4-C5-C6	5.49	119.74	117.00
26	BA	2247	A	N9-C4-C5	5.49	107.99	105.80
26	BA	2471	A	N9-C4-C5	5.49	107.99	105.80
26	BA	2882	A	N9-C4-C5	5.49	107.99	105.80
27	BB	52	A	N9-C4-C5	5.49	108.00	105.80
27	BB	78	A	C4-C5-C6	5.49	119.74	117.00
1	AA	151	A	N3-C4-N9	5.48	131.79	127.40
1	AA	520	A	C8-N9-C4	5.48	107.99	105.80
1	AA	766	A	N3-C4-N9	5.48	131.79	127.40
1	AA	1238	A	N3-C4-N9	5.48	131.79	127.40
26	BA	1419	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	1608	A	C8-N9-C4	5.48	107.99	105.80
26	BA	2142	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	28	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	792	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	1046	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	1333	A	C4-C5-C6	5.48	119.74	117.00
23	AW	23	A	C8-N9-C4	5.48	107.99	105.80
26	BA	127	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	362	A	C8-N9-C4	5.48	107.99	105.80
26	BA	432	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	716	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	749	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	896	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	1230	A	N9-C4-C5	5.48	107.99	105.80
26	BA	1586	A	N9-C4-C5	5.48	107.99	105.80
26	BA	1785	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	1786	A	N9-C4-C5	5.48	107.99	105.80
26	BA	1969	A	C4-C5-N7	-5.48	107.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2033	A	C8-N9-C4	5.48	107.99	105.80
26	BA	2809	A	N9-C4-C5	5.48	107.99	105.80
27	BB	104	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	50	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	129	A	C8-N9-C4	5.48	107.99	105.80
1	AA	743	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	780	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	1269	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	19	A	N9-C4-C5	5.48	107.99	105.80
26	BA	111	A	C8-N9-C4	5.48	107.99	105.80
26	BA	478	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	716	A	C8-N9-C4	5.48	107.99	105.80
26	BA	1067	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	1918	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	2727	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	2750	A	N9-C4-C5	5.48	107.99	105.80
1	AA	1476	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	1008	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	2614	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	59	A	N9-C4-C5	5.48	107.99	105.80
1	AA	228	A	N9-C4-C5	5.48	107.99	105.80
1	AA	415	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	767	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	1067	A	N9-C4-C5	5.48	107.99	105.80
1	AA	1480	A	N9-C4-C5	5.48	107.99	105.80
26	BA	19	A	C8-N9-C4	5.48	107.99	105.80
26	BA	310	A	N9-C4-C5	5.48	107.99	105.80
26	BA	472	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	621	A	C8-N9-C4	5.48	107.99	105.80
26	BA	735	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	1580	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	2020	A	C8-N9-C4	5.48	107.99	105.80
26	BA	2887	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	26	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	766	A	C4-C5-C6	5.48	119.74	117.00
1	AA	1288	A	N9-C4-C5	5.48	107.99	105.80
26	BA	877	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	878	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	1129	A	C8-N9-C4	5.48	107.99	105.80
26	BA	1194	A	C8-N9-C4	5.48	107.99	105.80
26	BA	1274	A	C4-C5-N7	-5.48	107.96	110.70
26	BA	1616	A	C4-C5-N7	-5.48	107.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	143	A	N9-C4-C5	5.47	107.99	105.80
1	AA	192	A	C8-N9-C4	5.47	107.99	105.80
1	AA	493	A	N9-C4-C5	5.47	107.99	105.80
1	AA	560	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	706	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	787	A	C8-N9-C4	5.47	107.99	105.80
1	AA	1093	A	C8-N9-C4	5.47	107.99	105.80
1	AA	1117	A	N9-C4-C5	5.47	107.99	105.80
1	AA	1357	A	C8-N9-C4	5.47	107.99	105.80
26	BA	354	A	N3-C4-N9	5.47	131.78	127.40
26	BA	478	A	N9-C4-C5	5.47	107.99	105.80
26	BA	849	A	C8-N9-C4	5.47	107.99	105.80
26	BA	972	A	C8-N9-C4	5.47	107.99	105.80
26	BA	983	A	N9-C4-C5	5.47	107.99	105.80
26	BA	1103	A	C4-C5-N7	-5.47	107.96	110.70
26	BA	1597	A	C8-N9-C4	5.47	107.99	105.80
26	BA	1802	A	C4-C5-N7	-5.47	107.96	110.70
26	BA	2033	A	C4-C5-C6	5.47	119.74	117.00
1	AA	10	A	N9-C4-C5	5.47	107.99	105.80
1	AA	199	A	N9-C4-C5	5.47	107.99	105.80
1	AA	246	A	N9-C4-C5	5.47	107.99	105.80
1	AA	274	A	N9-C4-C5	5.47	107.99	105.80
1	AA	768	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	777	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	918	A	C8-N9-C4	5.47	107.99	105.80
26	BA	95	A	C4-C5-N7	-5.47	107.96	110.70
26	BA	222	A	C4-C5-N7	-5.47	107.96	110.70
26	BA	340	A	C4-C5-N7	-5.47	107.96	110.70
26	BA	574	A	N3-C4-N9	5.47	131.78	127.40
26	BA	735	A	C8-N9-C4	5.47	107.99	105.80
26	BA	1634	A	C4-C5-N7	-5.47	107.96	110.70
26	BA	1785	A	C8-N9-C4	5.47	107.99	105.80
26	BA	1847	A	N9-C4-C5	5.47	107.99	105.80
26	BA	2163	A	C8-N9-C4	5.47	107.99	105.80
26	BA	2534	A	N9-C4-C5	5.47	107.99	105.80
1	AA	816	A	C8-N9-C4	5.47	107.99	105.80
1	AA	1238	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	522	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	602	A	N9-C4-C5	5.47	107.99	105.80
26	BA	626	A	C4-C5-N7	-5.47	107.96	110.70
26	BA	1020	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	1029	A	C8-N9-C4	5.47	107.99	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1127	A	C8-N9-C4	5.47	107.99	105.80
26	BA	1413	A	C4-C5-N7	-5.47	107.96	110.70
26	BA	1431	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	1690	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	2119	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	288	A	N9-C4-C5	5.47	107.99	105.80
1	AA	338	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	663	A	C8-N9-C4	5.47	107.99	105.80
1	AA	1275	A	N9-C4-C5	5.47	107.99	105.80
23	AW	69	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	10	A	C8-N9-C4	5.47	107.99	105.80
26	BA	152	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	1237	A	N9-C4-C5	5.47	107.99	105.80
26	BA	1367	A	N9-C4-C5	5.47	107.99	105.80
26	BA	1572	A	C8-N9-C4	5.47	107.99	105.80
26	BA	1614	A	C8-N9-C4	5.47	107.99	105.80
26	BA	1927	A	N9-C4-C5	5.47	107.99	105.80
26	BA	1970	A	C8-N9-C4	5.47	107.99	105.80
26	BA	2706	A	C8-N9-C4	5.47	107.99	105.80
1	AA	197	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	547	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	1503	A	N9-C4-C5	5.47	107.99	105.80
26	BA	472	A	C8-N9-C4	5.47	107.99	105.80
26	BA	973	A	N9-C4-C5	5.47	107.99	105.80
26	BA	1214	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	1419	A	C4-C5-C6	5.47	119.73	117.00
26	BA	1919	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	2886	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	2900	A	C8-N9-C4	5.47	107.99	105.80
1	AA	573	A	C8-N9-C4	5.47	107.99	105.80
1	AA	1042	A	C8-N9-C4	5.47	107.99	105.80
26	BA	13	A	C8-N9-C4	5.47	107.99	105.80
26	BA	900	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	927	A	N9-C4-C5	5.47	107.99	105.80
26	BA	945	A	N9-C4-C5	5.47	107.99	105.80
26	BA	1469	A	N9-C4-C5	5.47	107.99	105.80
26	BA	1938	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	2014	A	C8-N9-C4	5.47	107.99	105.80
26	BA	2031	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	2453	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	2639	A	C4-C5-N7	-5.47	107.97	110.70
26	BA	2821	A	N9-C4-C5	5.47	107.99	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	906	A	N9-C4-C5	5.46	107.99	105.80
1	AA	1036	A	C8-N9-C4	5.46	107.99	105.80
1	AA	1082	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1250	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1333	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1377	A	N9-C4-C5	5.46	107.99	105.80
23	AW	58	A	C8-N9-C4	5.46	107.99	105.80
26	BA	666	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	676	A	C8-N9-C4	5.46	107.99	105.80
26	BA	1285	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1494	A	N9-C4-C5	5.46	107.99	105.80
26	BA	1509	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1596	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1773	A	N9-C4-C5	5.46	107.99	105.80
26	BA	1932	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	2205	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	2478	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	2518	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	2670	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	171	A	N3-C4-N9	5.46	131.77	127.40
1	AA	182	A	C8-N9-C4	5.46	107.98	105.80
1	AA	777	A	N9-C4-C5	5.46	107.98	105.80
1	AA	1150	A	C8-N9-C4	5.46	107.98	105.80
1	AA	1216	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1239	A	C4-C5-N7	-5.46	107.97	110.70
24	AX	58	A	N9-C4-C5	5.46	107.98	105.80
26	BA	348	A	N9-C4-C5	5.46	107.98	105.80
26	BA	1040	A	N3-C4-N9	5.46	131.77	127.40
26	BA	1067	A	N9-C4-C5	5.46	107.98	105.80
26	BA	2418	A	N3-C4-N9	5.46	131.77	127.40
27	BB	58	A	N9-C4-C5	5.46	107.98	105.80
1	AA	189	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	459	A	N9-C4-C5	5.46	107.98	105.80
1	AA	640	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	706	A	N9-C4-C5	5.46	107.98	105.80
1	AA	715	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1349	A	N9-C4-C5	5.46	107.98	105.80
1	AA	1534	A	C4-C5-N7	-5.46	107.97	110.70
25	AY	23	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	42	A	N9-C4-C5	5.46	107.98	105.80
26	BA	144	A	N9-C4-C5	5.46	107.98	105.80
26	BA	716	A	N9-C4-C5	5.46	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	753	A	C8-N9-C4	5.46	107.98	105.80
26	BA	1027	A	N9-C4-C5	5.46	107.98	105.80
26	BA	1532	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1616	A	N9-C4-C5	5.46	107.98	105.80
26	BA	1739	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1966	A	C8-N9-C4	5.46	107.98	105.80
27	BB	99	A	C8-N9-C4	5.46	107.98	105.80
23	AW	69	A	C8-N9-C4	5.46	107.98	105.80
26	BA	101	A	N9-C4-C5	5.46	107.98	105.80
26	BA	911	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	2426	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	303	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	448	A	N9-C4-C5	5.46	107.98	105.80
1	AA	909	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1111	A	N9-C4-C5	5.46	107.98	105.80
1	AA	1274	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1430	A	C8-N9-C4	5.46	107.98	105.80
25	AY	35	A	C4-C5-N7	-5.46	107.97	110.70
25	AY	58	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	176	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	477	A	N9-C4-C5	5.46	107.98	105.80
26	BA	627	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	721	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1027	A	C8-N9-C4	5.46	107.98	105.80
26	BA	1439	A	N9-C4-C5	5.46	107.98	105.80
26	BA	1637	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1650	A	C8-N9-C4	5.46	107.98	105.80
26	BA	1654	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	2135	A	N9-C4-C5	5.46	107.98	105.80
26	BA	2270	A	N9-C4-C5	5.46	107.98	105.80
26	BA	2434	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	2781	A	C8-N9-C4	5.46	107.98	105.80
1	AA	19	A	C8-N9-C4	5.46	107.98	105.80
1	AA	298	A	N9-C4-C5	5.46	107.98	105.80
1	AA	412	A	N9-C4-C5	5.46	107.98	105.80
1	AA	459	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	630	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1483	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	103	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	219	A	C8-N9-C4	5.46	107.98	105.80
26	BA	340	A	N9-C4-C5	5.46	107.98	105.80
26	BA	983	A	C4-C5-N7	-5.46	107.97	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1420	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1819	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1952	A	N9-C4-C5	5.46	107.98	105.80
26	BA	1966	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	2448	A	N9-C4-C5	5.46	107.98	105.80
1	AA	520	A	N9-C4-C5	5.46	107.98	105.80
1	AA	1000	A	C8-N9-C4	5.46	107.98	105.80
26	BA	439	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1096	A	C8-N9-C4	5.46	107.98	105.80
26	BA	1272	A	N9-C4-C5	5.46	107.98	105.80
26	BA	1365	A	C4-C5-N7	-5.46	107.97	110.70
26	BA	1378	A	C8-N9-C4	5.46	107.98	105.80
27	BB	108	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	831	A	C8-N9-C4	5.45	107.98	105.80
1	AA	1019	A	N9-C4-C5	5.45	107.98	105.80
1	AA	1287	A	N9-C4-C5	5.45	107.98	105.80
26	BA	429	A	N9-C4-C5	5.45	107.98	105.80
26	BA	443	A	C8-N9-C4	5.45	107.98	105.80
26	BA	925	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	1285	A	C8-N9-C4	5.45	107.98	105.80
26	BA	1413	A	N9-C4-C5	5.45	107.98	105.80
26	BA	1552	A	N9-C4-C5	5.45	107.98	105.80
26	BA	1579	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	1598	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	1689	A	N9-C4-C5	5.45	107.98	105.80
26	BA	1858	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	2407	A	C8-N9-C4	5.45	107.98	105.80
1	AA	704	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	784	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	1067	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	1110	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	670	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	1254	A	N9-C4-C5	5.45	107.98	105.80
26	BA	1789	A	N9-C4-C5	5.45	107.98	105.80
26	BA	1912	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	1912	A	N9-C4-C5	5.45	107.98	105.80
26	BA	2565	A	C8-N9-C4	5.45	107.98	105.80
1	AA	77	A	N9-C4-C5	5.45	107.98	105.80
1	AA	101	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	306	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	574	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	629	A	C4-C5-N7	-5.45	107.97	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	794	A	N9-C4-C5	5.45	107.98	105.80
1	AA	1016	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	1254	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	1271	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	104	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	207	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	504	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	764	A	N9-C4-C5	5.45	107.98	105.80
26	BA	979	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	1189	A	N9-C4-C5	5.45	107.98	105.80
26	BA	1469	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	1608	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	1640	A	C8-N9-C4	5.45	107.98	105.80
26	BA	2366	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	2497	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	2766	A	C8-N9-C4	5.45	107.98	105.80
1	AA	26	A	C4-C5-C6	5.45	119.72	117.00
1	AA	498	A	C4-C5-N7	-5.45	107.98	110.70
1	AA	831	A	N9-C4-C5	5.45	107.98	105.80
26	BA	126	A	N9-C4-C5	5.45	107.98	105.80
26	BA	1080	A	C4-C5-N7	-5.45	107.98	110.70
26	BA	1890	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	2386	A	C8-N9-C4	5.45	107.98	105.80
26	BA	2665	A	C4-C5-N7	-5.45	107.97	110.70
26	BA	2809	A	C4-C5-N7	-5.45	107.98	110.70
1	AA	298	A	C4-C5-N7	-5.45	107.98	110.70
26	BA	1028	A	N9-C4-C5	5.45	107.98	105.80
26	BA	1264	A	N9-C4-C5	5.45	107.98	105.80
26	BA	1353	A	N9-C4-C5	5.45	107.98	105.80
26	BA	2733	A	C4-C5-N7	-5.45	107.98	110.70
1	AA	179	A	C8-N9-C4	5.45	107.98	105.80
1	AA	845	A	N9-C4-C5	5.45	107.98	105.80
1	AA	1257	A	C4-C5-N7	-5.45	107.98	110.70
26	BA	5	A	C8-N9-C4	5.45	107.98	105.80
26	BA	44	A	C4-C5-N7	-5.45	107.98	110.70
26	BA	1353	A	C4-C5-N7	-5.45	107.98	110.70
26	BA	2183	A	N9-C4-C5	5.45	107.98	105.80
26	BA	2566	A	N9-C4-C5	5.45	107.98	105.80
26	BA	2654	A	C4-C5-N7	-5.45	107.98	110.70
26	BA	2721	A	C4-C5-N7	-5.45	107.98	110.70
26	BA	2813	A	C4-C5-N7	-5.45	107.98	110.70
1	AA	344	A	N9-C4-C5	5.44	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1146	A	N9-C4-C5	5.44	107.98	105.80
1	AA	1499	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	892	A	C8-N9-C4	5.44	107.98	105.80
26	BA	933	A	C8-N9-C4	5.44	107.98	105.80
26	BA	2721	A	N9-C4-C5	5.44	107.98	105.80
26	BA	2741	A	C4-C5-N7	-5.44	107.98	110.70
27	BB	109	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	321	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	344	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	371	A	N9-C4-C5	5.44	107.98	105.80
1	AA	675	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	718	A	C4-C5-N7	-5.44	107.98	110.70
23	AW	31	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	14	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	368	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	423	A	N9-C4-C5	5.44	107.98	105.80
26	BA	1439	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	1655	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	1889	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	1998	A	C8-N9-C4	5.44	107.98	105.80
26	BA	2327	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	1151	A	N3-C4-N9	5.44	131.75	127.40
1	AA	1394	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	1456	A	C4-C5-N7	-5.44	107.98	110.70
25	AY	14	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	5	A	N9-C4-C5	5.44	107.98	105.80
26	BA	423	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	614	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	721	A	C8-N9-C4	5.44	107.98	105.80
26	BA	792	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	1403	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	1525	A	C8-N9-C4	5.44	107.98	105.80
26	BA	1805	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	2346	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	892	A	N9-C4-C5	5.44	107.98	105.80
1	AA	1502	A	C4-C5-N7	-5.44	107.98	110.70
23	AW	38	A	N9-C4-C5	5.44	107.97	105.80
23	AW	76	A	C8-N9-C4	5.44	107.98	105.80
26	BA	182	A	C8-N9-C4	5.44	107.98	105.80
26	BA	190	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	502	A	N9-C4-C5	5.44	107.98	105.80
26	BA	899	A	N9-C4-C5	5.44	107.97	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1213	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	1977	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	2542	A	N9-C4-C5	5.44	107.98	105.80
26	BA	2781	A	N9-C4-C5	5.44	107.98	105.80
1	AA	2	A	N9-C4-C5	5.44	107.97	105.80
1	AA	7	A	N9-C4-C5	5.44	107.97	105.80
1	AA	149	A	C8-N9-C4	5.44	107.97	105.80
1	AA	478	A	C8-N9-C4	5.44	107.97	105.80
1	AA	787	A	N9-C4-C5	5.44	107.97	105.80
1	AA	1429	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	1447	A	C4-C5-N7	-5.44	107.98	110.70
23	AW	59	A	N9-C4-C5	5.44	107.97	105.80
26	BA	73	A	N9-C4-C5	5.44	107.97	105.80
26	BA	984	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	1189	A	C8-N9-C4	5.44	107.97	105.80
26	BA	1571	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	1609	A	N9-C4-C5	5.44	107.97	105.80
26	BA	1640	A	N9-C4-C5	5.44	107.97	105.80
26	BA	1932	A	N9-C4-C5	5.44	107.97	105.80
26	BA	1966	A	N9-C4-C5	5.44	107.97	105.80
26	BA	2497	A	C8-N9-C4	5.44	107.97	105.80
1	AA	768	A	N9-C4-C5	5.44	107.97	105.80
1	AA	1271	A	N9-C4-C5	5.44	107.97	105.80
1	AA	1434	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	320	A	N9-C4-C5	5.44	107.97	105.80
26	BA	844	A	N9-C4-C5	5.44	107.97	105.80
26	BA	1632	A	N9-C4-C5	5.44	107.97	105.80
26	BA	1705	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	2635	A	C8-N9-C4	5.44	107.97	105.80
26	BA	2820	A	C4-C5-N7	-5.44	107.98	110.70
26	BA	2860	A	C8-N9-C4	5.44	107.97	105.80
1	AA	65	A	N9-C4-C5	5.43	107.97	105.80
1	AA	72	A	N9-C4-C5	5.43	107.97	105.80
1	AA	274	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	382	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	523	A	C8-N9-C4	5.43	107.97	105.80
1	AA	554	A	C8-N9-C4	5.43	107.97	105.80
1	AA	595	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	635	A	C8-N9-C4	5.43	107.97	105.80
1	AA	790	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	816	A	N9-C4-C5	5.43	107.97	105.80
1	AA	959	A	N9-C4-C5	5.43	107.97	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	969	A	N9-C4-C5	5.43	107.97	105.80
1	AA	1256	A	C4-C5-N7	-5.43	107.98	110.70
22	AV	15	A	C4-C5-N7	-5.43	107.98	110.70
23	AW	9	A	C8-N9-C4	5.43	107.97	105.80
26	BA	429	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	449	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	492	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	547	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	590	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	668	A	N3-C4-N9	5.43	131.75	127.40
26	BA	973	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	1054	A	N9-C4-C5	5.43	107.97	105.80
26	BA	1453	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	1569	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	2042	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	2278	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	2469	A	N3-C4-N9	5.43	131.75	127.40
26	BA	2482	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	2705	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	2778	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	155	A	N9-C4-C5	5.43	107.97	105.80
1	AA	509	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	539	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	860	A	N9-C4-C5	5.43	107.97	105.80
1	AA	946	A	N9-C4-C5	5.43	107.97	105.80
1	AA	1004	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	64	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	497	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	699	A	C8-N9-C4	5.43	107.97	105.80
26	BA	718	A	N9-C4-C5	5.43	107.97	105.80
26	BA	844	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	1039	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	1126	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	1142	A	N9-C4-C5	5.43	107.97	105.80
26	BA	1569	A	N9-C4-C5	5.43	107.97	105.80
26	BA	2317	A	N9-C4-C5	5.43	107.97	105.80
26	BA	2572	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	151	A	C8-N9-C4	5.43	107.97	105.80
22	AV	17	A	N9-C4-C5	5.43	107.97	105.80
26	BA	203	A	N9-C4-C5	5.43	107.97	105.80
26	BA	507	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	609	A	C4-C5-N7	-5.43	107.98	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	715	A	N9-C4-C5	5.43	107.97	105.80
26	BA	781	A	N9-C4-C5	5.43	107.97	105.80
26	BA	1126	A	N9-C4-C5	5.43	107.97	105.80
26	BA	1144	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	1147	A	N3-C4-N9	5.43	131.75	127.40
1	AA	364	A	N9-C4-C5	5.43	107.97	105.80
1	AA	1163	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	1169	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	1332	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	1518	A	C4-C5-N7	-5.43	107.98	110.70
25	AY	21	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	981	A	C8-N9-C4	5.43	107.97	105.80
26	BA	1085	A	C4-C5-N7	-5.43	107.98	110.70
26	BA	1151	A	C4-C5-N7	-5.43	107.99	110.70
26	BA	1384	A	N9-C4-C5	5.43	107.97	105.80
26	BA	1544	A	N9-C4-C5	5.43	107.97	105.80
26	BA	1598	A	C8-N9-C4	5.43	107.97	105.80
26	BA	1877	A	N9-C4-C5	5.43	107.97	105.80
26	BA	2052	A	N9-C4-C5	5.43	107.97	105.80
26	BA	2893	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	621	A	C4-C5-N7	-5.43	107.99	110.70
26	BA	877	A	N9-C4-C5	5.43	107.97	105.80
26	BA	943	A	C4-C5-N7	-5.43	107.99	110.70
26	BA	947	A	C4-C5-N7	-5.43	107.99	110.70
26	BA	1953	A	N3-C4-N9	5.43	131.74	127.40
26	BA	2809	A	C8-N9-C4	5.43	107.97	105.80
27	BB	53	A	N9-C4-C5	5.43	107.97	105.80
27	BB	94	A	N9-C4-C5	5.43	107.97	105.80
27	BB	101	A	N9-C4-C5	5.43	107.97	105.80
1	AA	77	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	109	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	262	A	N9-C4-C5	5.43	107.97	105.80
1	AA	279	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	303	A	N9-C4-C5	5.43	107.97	105.80
1	AA	315	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	938	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	1152	A	C8-N9-C4	5.43	107.97	105.80
1	AA	1179	A	N9-C4-C5	5.43	107.97	105.80
1	AA	1250	A	N9-C4-C5	5.43	107.97	105.80
23	AW	26	A	N9-C4-C5	5.43	107.97	105.80
26	BA	6	A	C8-N9-C4	5.43	107.97	105.80
26	BA	165	A	C8-N9-C4	5.43	107.97	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	866	A	C4-C5-N7	-5.43	107.99	110.70
26	BA	1089	A	N9-C4-C5	5.43	107.97	105.80
26	BA	1129	A	C4-C5-N7	-5.43	107.99	110.70
26	BA	1175	A	N9-C4-C5	5.43	107.97	105.80
26	BA	1433	A	N9-C4-C5	5.43	107.97	105.80
26	BA	1528	A	C4-C5-N7	-5.43	107.99	110.70
26	BA	1593	A	N9-C4-C5	5.43	107.97	105.80
26	BA	1650	A	C4-C5-N7	-5.43	107.99	110.70
26	BA	2019	A	N3-C4-N9	5.43	131.74	127.40
26	BA	2071	A	N9-C4-C5	5.43	107.97	105.80
26	BA	2170	A	N9-C4-C5	5.43	107.97	105.80
26	BA	2476	A	C4-C5-N7	-5.43	107.99	110.70
26	BA	2711	A	C8-N9-C4	5.43	107.97	105.80
26	BA	2900	A	N9-C4-C5	5.43	107.97	105.80
1	AA	554	A	N3-C4-N9	5.42	131.74	127.40
1	AA	602	A	N9-C4-C5	5.42	107.97	105.80
1	AA	635	A	N9-C4-C5	5.42	107.97	105.80
1	AA	665	A	C8-N9-C4	5.42	107.97	105.80
1	AA	665	A	N3-C4-N9	5.42	131.74	127.40
1	AA	865	A	C8-N9-C4	5.42	107.97	105.80
1	AA	1080	A	C4-C5-N7	-5.42	107.99	110.70
23	AW	73	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	309	A	N9-C4-C5	5.42	107.97	105.80
26	BA	556	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	734	A	N9-C4-C5	5.42	107.97	105.80
26	BA	756	A	C8-N9-C4	5.42	107.97	105.80
26	BA	764	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	892	A	N9-C4-C5	5.42	107.97	105.80
26	BA	1169	A	N9-C4-C5	5.42	107.97	105.80
26	BA	1608	A	N9-C4-C5	5.42	107.97	105.80
26	BA	1701	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	2205	A	N9-C4-C5	5.42	107.97	105.80
26	BA	2670	A	N9-C4-C5	5.42	107.97	105.80
26	BA	2700	A	C4-C5-N7	-5.42	107.99	110.70
27	BB	59	A	C8-N9-C4	5.42	107.97	105.80
1	AA	119	A	N9-C4-C5	5.42	107.97	105.80
1	AA	766	A	C8-N9-C4	5.42	107.97	105.80
1	AA	1197	A	N9-C4-C5	5.42	107.97	105.80
26	BA	181	A	N9-C4-C5	5.42	107.97	105.80
26	BA	221	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	311	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	563	A	C4-C5-N7	-5.42	107.99	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	917	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	2042	A	N9-C4-C5	5.42	107.97	105.80
26	BA	2095	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	197	A	N9-C4-C5	5.42	107.97	105.80
1	AA	338	A	N9-C4-C5	5.42	107.97	105.80
1	AA	460	A	N9-C4-C5	5.42	107.97	105.80
1	AA	468	A	C8-N9-C4	5.42	107.97	105.80
1	AA	630	A	N9-C4-C5	5.42	107.97	105.80
25	AY	26	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	404	A	C8-N9-C4	5.42	107.97	105.80
26	BA	1155	A	C8-N9-C4	5.42	107.97	105.80
26	BA	1665	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	1679	A	N9-C4-C5	5.42	107.97	105.80
26	BA	2176	A	C8-N9-C4	5.42	107.97	105.80
26	BA	2199	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	2199	A	N9-C4-C5	5.42	107.97	105.80
26	BA	2602	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	2639	A	N9-C4-C5	5.42	107.97	105.80
26	BA	2810	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	393	A	N3-C4-N9	5.42	131.74	127.40
1	AA	535	A	N9-C4-C5	5.42	107.97	105.80
1	AA	622	A	N3-C4-N9	5.42	131.74	127.40
24	AX	76	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	374	A	N9-C4-C5	5.42	107.97	105.80
26	BA	1722	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	1808	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	2212	A	C4-C5-N7	-5.42	107.99	110.70
27	BB	57	A	C8-N9-C4	5.42	107.97	105.80
1	AA	190	A	C8-N9-C4	5.42	107.97	105.80
1	AA	560	A	N9-C4-C5	5.42	107.97	105.80
1	AA	968	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	1150	A	N3-C4-N9	5.42	131.73	127.40
1	AA	1288	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	514	A	C4-C5-C6	5.42	119.71	117.00
26	BA	590	A	N9-C4-C5	5.42	107.97	105.80
26	BA	616	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	1020	A	N9-C4-C5	5.42	107.97	105.80
26	BA	1264	A	C8-N9-C4	5.42	107.97	105.80
26	BA	1690	A	N9-C4-C5	5.42	107.97	105.80
26	BA	1802	A	N9-C4-C5	5.42	107.97	105.80
26	BA	1918	A	N9-C4-C5	5.42	107.97	105.80
26	BA	2503	A	N9-C4-C5	5.42	107.97	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2660	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	2740	A	C8-N9-C4	5.42	107.97	105.80
27	BB	99	A	N9-C4-C5	5.42	107.97	105.80
1	AA	172	A	N9-C4-C5	5.42	107.97	105.80
1	AA	315	A	N9-C4-C5	5.42	107.97	105.80
1	AA	676	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	715	A	N9-C4-C5	5.42	107.97	105.80
1	AA	1285	A	C4-C5-N7	-5.42	107.99	110.70
24	AX	21	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	74	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	231	A	N9-C4-C5	5.42	107.97	105.80
26	BA	324	A	N9-C4-C5	5.42	107.97	105.80
26	BA	575	A	N9-C4-C5	5.42	107.97	105.80
26	BA	753	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	1048	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	1088	A	C8-N9-C4	5.42	107.97	105.80
26	BA	1090	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	1679	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	2679	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	203	A	C4-C5-N7	-5.42	107.99	110.70
26	BA	429	A	C8-N9-C4	5.42	107.97	105.80
26	BA	1525	A	N9-C4-C5	5.42	107.97	105.80
26	BA	1676	A	C8-N9-C4	5.42	107.97	105.80
26	BA	2412	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	468	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	702	A	N9-C4-C5	5.41	107.97	105.80
1	AA	747	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	873	A	C4-C5-N7	-5.41	107.99	110.70
26	BA	213	A	C4-C5-N7	-5.41	107.99	110.70
26	BA	347	A	N9-C4-C5	5.41	107.97	105.80
26	BA	391	A	C4-C5-N7	-5.41	107.99	110.70
26	BA	981	A	N9-C4-C5	5.41	107.97	105.80
26	BA	1264	A	C4-C5-N7	-5.41	107.99	110.70
26	BA	2497	A	N9-C4-C5	5.41	107.97	105.80
27	BB	46	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	174	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	539	A	N9-C4-C5	5.41	107.97	105.80
1	AA	1340	A	C4-C5-N7	-5.41	107.99	110.70
26	BA	125	A	N9-C4-C5	5.41	107.97	105.80
26	BA	443	A	C4-C5-N7	-5.41	107.99	110.70
26	BA	627	A	N9-C4-C5	5.41	107.97	105.80
26	BA	1419	A	C8-N9-C4	5.41	107.97	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2134	A	C8-N9-C4	5.41	107.97	105.80
26	BA	2227	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	465	A	N9-C4-C5	5.41	107.96	105.80
1	AA	466	A	N9-C4-C5	5.41	107.96	105.80
1	AA	728	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	807	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	901	A	N9-C4-C5	5.41	107.96	105.80
1	AA	908	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1188	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	1306	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1339	A	C4-C5-N7	-5.41	108.00	110.70
25	AY	58	A	N9-C4-C5	5.41	107.96	105.80
26	BA	199	A	N9-C4-C5	5.41	107.97	105.80
26	BA	279	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	1073	A	N9-C4-C5	5.41	107.96	105.80
26	BA	1133	A	N9-C4-C5	5.41	107.96	105.80
26	BA	1701	A	N9-C4-C5	5.41	107.96	105.80
26	BA	2059	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2059	A	N9-C4-C5	5.41	107.96	105.80
26	BA	2309	A	N9-C4-C5	5.41	107.97	105.80
26	BA	2358	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2433	A	C4-C5-N7	-5.41	107.99	110.70
26	BA	2883	A	C4-C5-N7	-5.41	108.00	110.70
27	BB	59	A	C5-C6-N1	5.41	120.41	117.70
1	AA	167	A	N9-C4-C5	5.41	107.96	105.80
1	AA	263	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	907	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1171	A	N9-C4-C5	5.41	107.96	105.80
1	AA	1299	A	C8-N9-C4	5.41	107.96	105.80
1	AA	1437	A	N9-C4-C5	5.41	107.96	105.80
26	BA	195	A	N9-C4-C5	5.41	107.96	105.80
26	BA	428	A	N9-C4-C5	5.41	107.96	105.80
26	BA	654	A	C8-N9-C4	5.41	107.96	105.80
26	BA	1028	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	1328	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	1495	A	C8-N9-C4	5.41	107.96	105.80
26	BA	1504	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	1978	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2369	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2450	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2682	A	N9-C4-C5	5.41	107.96	105.80
26	BA	2706	A	C4-C5-N7	-5.41	108.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BB	66	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	374	A	N9-C4-C5	5.41	107.96	105.80
1	AA	579	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	270	A	N9-C4-C5	5.41	107.96	105.80
26	BA	346	A	N9-C4-C5	5.41	107.96	105.80
26	BA	1133	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	1384	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	1876	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2284	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2317	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2781	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	412	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1170	A	N3-C4-N9	5.41	131.72	127.40
1	AA	1269	A	C8-N9-C4	5.41	107.96	105.80
25	AY	69	A	N9-C4-C5	5.41	107.96	105.80
26	BA	213	A	N9-C4-C5	5.41	107.96	105.80
26	BA	470	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	996	A	N9-C4-C5	5.41	107.96	105.80
26	BA	1226	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	1365	A	N9-C4-C5	5.41	107.96	105.80
26	BA	1490	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	1937	A	N3-C4-N9	5.41	131.72	127.40
26	BA	2005	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2117	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2425	A	C4-C5-N7	-5.41	108.00	110.70
26	BA	2727	A	N9-C4-C5	5.41	107.96	105.80
27	BB	78	A	C8-N9-C4	5.41	107.96	105.80
26	BA	13	A	N9-C4-C5	5.40	107.96	105.80
26	BA	28	A	N9-C4-C5	5.40	107.96	105.80
26	BA	432	A	N9-C4-C5	5.40	107.96	105.80
26	BA	529	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	2434	A	C8-N9-C4	5.40	107.96	105.80
26	BA	2614	A	N9-C4-C5	5.40	107.96	105.80
26	BA	2635	A	N9-C4-C5	5.40	107.96	105.80
27	BB	104	A	N9-C4-C5	5.40	107.96	105.80
1	AA	336	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	412	A	C4-C5-C6	5.40	119.70	117.00
1	AA	441	A	N9-C4-C5	5.40	107.96	105.80
1	AA	1213	A	C4-C5-N7	-5.40	108.00	110.70
24	AX	9	A	N9-C4-C5	5.40	107.96	105.80
26	BA	161	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	197	A	C4-C5-N7	-5.40	108.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	256	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	1336	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	1383	A	C8-N9-C4	5.40	107.96	105.80
26	BA	2749	A	C4-C5-N7	-5.40	108.00	110.70
27	BB	15	A	C8-N9-C4	5.40	107.96	105.80
1	AA	784	A	N9-C4-C5	5.40	107.96	105.80
23	AW	21	A	N9-C4-C5	5.40	107.96	105.80
25	AY	41	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	167	A	N9-C4-C5	5.40	107.96	105.80
26	BA	505	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	722	A	N9-C4-C5	5.40	107.96	105.80
26	BA	980	A	N9-C4-C5	5.40	107.96	105.80
26	BA	1057	A	N9-C4-C5	5.40	107.96	105.80
26	BA	1495	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	1916	A	N9-C4-C5	5.40	107.96	105.80
26	BA	2005	A	N9-C4-C5	5.40	107.96	105.80
26	BA	2392	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	2810	A	N9-C4-C5	5.40	107.96	105.80
1	AA	172	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	448	A	C8-N9-C4	5.40	107.96	105.80
1	AA	913	A	N9-C4-C5	5.40	107.96	105.80
1	AA	1046	A	N9-C4-C5	5.40	107.96	105.80
25	AY	21	A	N9-C4-C5	5.40	107.96	105.80
26	BA	53	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	599	A	N9-C4-C5	5.40	107.96	105.80
26	BA	603	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	751	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	892	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	2589	A	N3-C4-N9	5.40	131.72	127.40
26	BA	2635	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	366	A	N9-C4-C5	5.40	107.96	105.80
1	AA	695	A	N9-C4-C5	5.40	107.96	105.80
1	AA	1171	A	C4-C5-N7	-5.40	108.00	110.70
23	AW	69	A	N9-C4-C5	5.40	107.96	105.80
26	BA	13	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	324	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	575	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	800	A	C4-C5-C6	5.40	119.70	117.00
26	BA	1626	A	N9-C4-C5	5.40	107.96	105.80
26	BA	2070	A	C8-N9-C4	5.40	107.96	105.80
26	BA	2346	A	N9-C4-C5	5.40	107.96	105.80
26	BA	2378	A	C4-C5-N7	-5.40	108.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2872	A	C8-N9-C4	5.40	107.96	105.80
27	BB	46	A	N9-C4-C5	5.40	107.96	105.80
1	AA	716	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	1470	A	C4-C5-N7	-5.40	108.00	110.70
26	BA	1495	A	N9-C4-C5	5.40	107.96	105.80
1	AA	81	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	1274	A	N9-C4-C5	5.39	107.96	105.80
1	AA	1433	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	1446	A	N9-C4-C5	5.39	107.96	105.80
26	BA	95	A	N9-C4-C5	5.39	107.96	105.80
26	BA	173	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	756	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	1050	A	N9-C4-C5	5.39	107.96	105.80
26	BA	1269	A	C8-N9-C4	5.39	107.96	105.80
26	BA	1393	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	1596	A	N9-C4-C5	5.39	107.96	105.80
26	BA	1635	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	1759	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	1871	A	N9-C4-C5	5.39	107.96	105.80
26	BA	2682	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	33	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	300	A	C8-N9-C4	5.39	107.96	105.80
24	AX	3	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	14	A	N9-C4-C5	5.39	107.96	105.80
26	BA	118	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	218	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	789	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	943	A	N9-C4-C5	5.39	107.96	105.80
26	BA	1039	A	N9-C4-C5	5.39	107.96	105.80
26	BA	1580	A	N9-C4-C5	5.39	107.96	105.80
26	BA	1749	A	N9-C4-C5	5.39	107.96	105.80
26	BA	2051	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	160	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	196	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	325	A	N9-C4-C5	5.39	107.96	105.80
1	AA	336	A	N9-C4-C5	5.39	107.96	105.80
1	AA	1431	A	N9-C4-C5	5.39	107.96	105.80
26	BA	666	A	N9-C4-C5	5.39	107.96	105.80
26	BA	1505	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	2733	A	N9-C4-C5	5.39	107.96	105.80
1	AA	182	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	787	A	C4-C5-N7	-5.39	108.01	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	38	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	661	A	N9-C4-C5	5.39	107.96	105.80
26	BA	706	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	783	A	C4-C5-N7	-5.39	108.00	110.70
26	BA	1545	A	C4-C5-C6	5.39	119.69	117.00
26	BA	1545	A	C4-C5-N7	-5.39	108.01	110.70
26	BA	2411	A	N9-C4-C5	5.39	107.96	105.80
26	BA	2757	A	C8-N9-C4	5.39	107.96	105.80
27	BB	73	A	C8-N9-C4	5.39	107.95	105.80
1	AA	1375	A	C4-C5-N7	-5.39	108.01	110.70
26	BA	233	A	C4-C5-N7	-5.39	108.01	110.70
26	BA	251	A	N9-C4-C5	5.39	107.95	105.80
26	BA	626	A	N9-C4-C5	5.39	107.95	105.80
26	BA	715	A	C8-N9-C4	5.39	107.95	105.80
26	BA	1287	A	N9-C4-C5	5.39	107.95	105.80
26	BA	1383	A	N9-C4-C5	5.39	107.95	105.80
27	BB	15	A	C4-C5-N7	-5.39	108.01	110.70
1	AA	195	A	C8-N9-C4	5.39	107.95	105.80
1	AA	706	A	C8-N9-C4	5.39	107.95	105.80
1	AA	900	A	N9-C4-C5	5.39	107.95	105.80
1	AA	1219	A	N9-C4-C5	5.39	107.95	105.80
26	BA	94	A	C4-C5-N7	-5.39	108.01	110.70
26	BA	344	A	N9-C4-C5	5.39	107.95	105.80
26	BA	670	A	N9-C4-C5	5.39	107.95	105.80
26	BA	829	A	N9-C4-C5	5.39	107.95	105.80
26	BA	1275	A	C4-C5-N7	-5.39	108.01	110.70
26	BA	1366	A	N9-C4-C5	5.39	107.95	105.80
26	BA	1566	A	N9-C4-C5	5.39	107.95	105.80
26	BA	1705	A	N9-C4-C5	5.39	107.95	105.80
26	BA	1735	A	C4-C5-N7	-5.39	108.01	110.70
26	BA	2184	A	C8-N9-C4	5.39	107.95	105.80
26	BA	2468	A	C4-C5-N7	-5.39	108.01	110.70
26	BA	2868	A	C4-C5-N7	-5.39	108.01	110.70
1	AA	397	A	C5-C6-N1	5.38	120.39	117.70
1	AA	460	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	493	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	780	A	C8-N9-C4	5.38	107.95	105.80
1	AA	935	A	C4-C5-N7	-5.38	108.01	110.70
22	AV	17	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	233	A	N9-C4-C5	5.38	107.95	105.80
26	BA	300	A	C8-N9-C4	5.38	107.95	105.80
26	BA	402	A	C4-C5-N7	-5.38	108.01	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	443	A	N9-C4-C5	5.38	107.95	105.80
26	BA	522	A	N9-C4-C5	5.38	107.95	105.80
26	BA	990	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	1073	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	1327	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	1901	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	2469	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	160	A	N9-C4-C5	5.38	107.95	105.80
1	AA	595	A	N9-C4-C5	5.38	107.95	105.80
1	AA	702	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1035	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	794	A	C4-C5-N7	-5.38	108.01	110.70
27	BB	39	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	71	A	N9-C4-C5	5.38	107.95	105.80
1	AA	1014	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1130	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	483	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	675	A	C8-N9-C4	5.38	107.95	105.80
26	BA	722	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	900	A	N9-C4-C5	5.38	107.95	105.80
26	BA	980	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	1505	A	N9-C4-C5	5.38	107.95	105.80
26	BA	1535	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	1890	A	N9-C4-C5	5.38	107.95	105.80
26	BA	2281	A	N9-C4-C5	5.38	107.95	105.80
26	BA	2376	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	2764	A	N3-C4-N9	5.38	131.71	127.40
1	AA	373	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	452	A	C8-N9-C4	5.38	107.95	105.80
1	AA	676	A	N9-C4-C5	5.38	107.95	105.80
1	AA	1299	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	161	A	C8-N9-C4	5.38	107.95	105.80
26	BA	878	A	N9-C4-C5	5.38	107.95	105.80
26	BA	928	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	1111	A	N9-C4-C5	5.38	107.95	105.80
26	BA	1434	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	2268	A	N9-C4-C5	5.38	107.95	105.80
26	BA	2758	A	N9-C4-C5	5.38	107.95	105.80
1	AA	411	A	C8-N9-C4	5.38	107.95	105.80
1	AA	498	A	N9-C4-C5	5.38	107.95	105.80
1	AA	520	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	729	A	N9-C4-C5	5.38	107.95	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	889	A	N3-C4-N9	5.38	131.70	127.40
1	AA	1004	A	N9-C4-C5	5.38	107.95	105.80
1	AA	1256	A	N9-C4-C5	5.38	107.95	105.80
1	AA	1430	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	226	A	N9-C4-C5	5.38	107.95	105.80
26	BA	322	A	N9-C4-C5	5.38	107.95	105.80
26	BA	404	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	412	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	792	A	N9-C4-C5	5.38	107.95	105.80
26	BA	960	A	N9-C4-C5	5.38	107.95	105.80
26	BA	1253	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	1359	A	N9-C4-C5	5.38	107.95	105.80
26	BA	1637	A	N9-C4-C5	5.38	107.95	105.80
26	BA	1650	A	N9-C4-C5	5.38	107.95	105.80
26	BA	1665	A	N9-C4-C5	5.38	107.95	105.80
26	BA	2433	A	N9-C4-C5	5.38	107.95	105.80
1	AA	2	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	430	A	N9-C4-C5	5.38	107.95	105.80
1	AA	975	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1236	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1508	A	C8-N9-C4	5.38	107.95	105.80
26	BA	44	A	N9-C4-C5	5.38	107.95	105.80
26	BA	515	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	821	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	1001	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	1385	A	N3-C4-N9	5.38	131.70	127.40
26	BA	1427	A	C4-C5-C6	5.38	119.69	117.00
26	BA	1566	A	C4-C5-N7	-5.38	108.01	110.70
26	BA	2119	A	N9-C4-C5	5.38	107.95	105.80
26	BA	2748	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	363	A	N9-C4-C5	5.38	107.95	105.80
1	AA	1201	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1418	A	N9-C4-C5	5.38	107.95	105.80
1	AA	1434	A	N9-C4-C5	5.38	107.95	105.80
24	AX	41	A	N9-C4-C5	5.38	107.95	105.80
26	BA	216	A	N9-C4-C5	5.38	107.95	105.80
26	BA	727	A	N9-C4-C5	5.38	107.95	105.80
26	BA	1336	A	N9-C4-C5	5.38	107.95	105.80
26	BA	1469	A	C8-N9-C4	5.38	107.95	105.80
26	BA	1522	A	N9-C4-C5	5.38	107.95	105.80
26	BA	2860	A	N9-C4-C5	5.38	107.95	105.80
1	AA	171	A	C4-C5-C6	5.37	119.69	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	250	A	C4-C5-N7	-5.37	108.01	110.70
1	AA	300	A	C4-C5-N7	-5.37	108.01	110.70
1	AA	461	A	N9-C4-C5	5.37	107.95	105.80
1	AA	499	A	C4-C5-C6	5.37	119.69	117.00
1	AA	994	A	C4-C5-N7	-5.37	108.01	110.70
1	AA	996	A	C4-C5-N7	-5.37	108.01	110.70
1	AA	1431	A	C4-C5-N7	-5.37	108.01	110.70
1	AA	1447	A	N9-C4-C5	5.37	107.95	105.80
26	BA	730	A	C4-C5-N7	-5.37	108.01	110.70
26	BA	756	A	N9-C4-C5	5.37	107.95	105.80
26	BA	866	A	N9-C4-C5	5.37	107.95	105.80
26	BA	941	A	C4-C5-N7	-5.37	108.01	110.70
26	BA	1321	A	C4-C5-N7	-5.37	108.01	110.70
26	BA	1433	A	C8-N9-C4	5.37	107.95	105.80
26	BA	1494	A	C8-N9-C4	5.37	107.95	105.80
26	BA	1735	A	N9-C4-C5	5.37	107.95	105.80
26	BA	2311	A	C4-C5-N7	-5.37	108.01	110.70
26	BA	2461	A	C4-C5-N7	-5.37	108.01	110.70
26	BA	2823	A	C8-N9-C4	5.37	107.95	105.80
1	AA	53	A	N9-C4-C5	5.37	107.95	105.80
1	AA	1251	A	N9-C4-C5	5.37	107.95	105.80
26	BA	64	A	N9-C4-C5	5.37	107.95	105.80
26	BA	146	A	C4-C5-N7	-5.37	108.01	110.70
26	BA	608	A	N9-C4-C5	5.37	107.95	105.80
26	BA	643	A	C4-C5-N7	-5.37	108.01	110.70
26	BA	677	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	1070	A	C4-C5-N7	-5.37	108.01	110.70
26	BA	1088	A	C4-C5-N7	-5.37	108.01	110.70
26	BA	1744	A	C4-C5-N7	-5.37	108.01	110.70
1	AA	596	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	978	A	N9-C4-C5	5.37	107.95	105.80
1	AA	1280	A	N9-C4-C5	5.37	107.95	105.80
1	AA	1396	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	761	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	1403	A	N9-C4-C5	5.37	107.95	105.80
26	BA	2003	A	N9-C4-C5	5.37	107.95	105.80
1	AA	539	A	C8-N9-C4	5.37	107.95	105.80
1	AA	743	A	N9-C4-C5	5.37	107.95	105.80
1	AA	819	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	1468	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	1500	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	56	A	C5-C6-N1	5.37	120.39	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1156	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	1551	A	N9-C4-C5	5.37	107.95	105.80
26	BA	1819	A	N9-C4-C5	5.37	107.95	105.80
26	BA	2212	A	N9-C4-C5	5.37	107.95	105.80
24	AX	14	A	N9-C4-C5	5.37	107.95	105.80
26	BA	905	A	N3-C4-N9	5.37	131.69	127.40
26	BA	2657	A	N9-C4-C5	5.37	107.95	105.80
26	BA	2837	A	N9-C4-C5	5.37	107.95	105.80
26	BA	2879	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	282	A	N9-C4-C5	5.37	107.95	105.80
1	AA	574	A	C8-N9-C4	5.37	107.95	105.80
1	AA	816	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	1340	A	N9-C4-C5	5.37	107.95	105.80
24	AX	23	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	272	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	322	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	661	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	1027	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	1509	A	N9-C4-C5	5.37	107.95	105.80
26	BA	1528	A	N9-C4-C5	5.37	107.95	105.80
26	BA	1780	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	1858	A	N9-C4-C5	5.37	107.95	105.80
26	BA	1885	A	C4-C5-N7	-5.37	108.02	110.70
26	BA	2020	A	N9-C4-C5	5.37	107.95	105.80
26	BA	2051	A	N9-C4-C5	5.37	107.95	105.80
26	BA	2060	A	N9-C4-C5	5.37	107.95	105.80
26	BA	2451	A	N3-C4-N9	5.37	131.69	127.40
26	BA	2837	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	28	A	N9-C4-C5	5.36	107.95	105.80
1	AA	98	A	C5-C6-N1	5.36	120.38	117.70
1	AA	415	A	N9-C4-C5	5.36	107.94	105.80
1	AA	792	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1092	A	C8-N9-C4	5.36	107.95	105.80
1	AA	1110	A	N9-C4-C5	5.36	107.95	105.80
1	AA	1180	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1446	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	71	A	N9-C4-C5	5.36	107.95	105.80
26	BA	311	A	N9-C4-C5	5.36	107.94	105.80
26	BA	676	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	751	A	N9-C4-C5	5.36	107.95	105.80
26	BA	820	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	1265	A	C4-C5-N7	-5.36	108.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1302	A	N9-C4-C5	5.36	107.94	105.80
26	BA	1571	A	N9-C4-C5	5.36	107.95	105.80
1	AA	468	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1430	A	N9-C4-C5	5.36	107.94	105.80
25	AY	14	A	N9-C4-C5	5.36	107.94	105.80
26	BA	226	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	675	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	1086	A	N9-C4-C5	5.36	107.94	105.80
26	BA	2705	A	N9-C4-C5	5.36	107.94	105.80
1	AA	116	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	116	A	N9-C4-C5	5.36	107.94	105.80
1	AA	716	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1188	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1227	A	C8-N9-C4	5.36	107.94	105.80
26	BA	342	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	1810	A	C8-N9-C4	5.36	107.94	105.80
26	BA	1900	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	2225	A	C8-N9-C4	5.36	107.94	105.80
26	BA	2278	A	N9-C4-C5	5.36	107.94	105.80
26	BA	2392	A	N9-C4-C5	5.36	107.94	105.80
26	BA	2726	A	N9-C4-C5	5.36	107.94	105.80
26	BA	2856	A	C4-C5-N7	-5.36	108.02	110.70
27	BB	108	A	N9-C4-C5	5.36	107.94	105.80
1	AA	32	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	1456	A	N9-C4-C5	5.36	107.94	105.80
26	BA	104	A	N9-C4-C5	5.36	107.94	105.80
26	BA	401	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	439	A	N9-C4-C5	5.36	107.94	105.80
26	BA	1805	A	N9-C4-C5	5.36	107.94	105.80
26	BA	1978	A	N9-C4-C5	5.36	107.94	105.80
26	BA	2587	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	2883	A	N9-C4-C5	5.36	107.94	105.80
1	AA	120	A	N9-C4-C5	5.36	107.94	105.80
1	AA	496	A	C8-N9-C4	5.36	107.94	105.80
1	AA	1145	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	282	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	1383	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	1626	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	1872	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	2126	A	N9-C4-C5	5.36	107.94	105.80
26	BA	2872	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	2873	A	C8-N9-C4	5.36	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BB	34	A	N3-C4-N9	5.36	131.69	127.40
1	AA	205	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	205	A	N9-C4-C5	5.36	107.94	105.80
1	AA	487	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	579	A	N9-C4-C5	5.36	107.94	105.80
1	AA	718	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1433	A	N9-C4-C5	5.36	107.94	105.80
23	AW	14	A	N9-C4-C5	5.36	107.94	105.80
26	BA	352	A	N9-C4-C5	5.36	107.94	105.80
26	BA	504	A	N9-C4-C5	5.36	107.94	105.80
26	BA	637	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	972	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	1009	A	C8-N9-C4	5.36	107.94	105.80
26	BA	1014	A	N3-C4-N9	5.36	131.69	127.40
26	BA	1373	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	1630	A	N3-C4-N9	5.36	131.69	127.40
26	BA	1744	A	N9-C4-C5	5.36	107.94	105.80
26	BA	1784	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	1801	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	1866	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	2062	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	2266	A	C4-C5-N7	-5.36	108.02	110.70
26	BA	2482	A	N9-C4-C5	5.36	107.94	105.80
27	BB	57	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	1101	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	1476	A	N9-C4-C5	5.35	107.94	105.80
26	BA	21	A	C4-C5-N7	-5.35	108.02	110.70
26	BA	972	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1713	A	C4-C5-N7	-5.35	108.02	110.70
26	BA	1739	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1854	A	N9-C4-C5	5.35	107.94	105.80
26	BA	2386	A	N9-C4-C5	5.35	107.94	105.80
1	AA	3	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	101	A	N9-C4-C5	5.35	107.94	105.80
1	AA	161	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	162	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	364	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	767	A	N9-C4-C5	5.35	107.94	105.80
1	AA	807	A	N9-C4-C5	5.35	107.94	105.80
1	AA	994	A	C8-N9-C4	5.35	107.94	105.80
1	AA	1081	A	C4-C5-N7	-5.35	108.02	110.70
26	BA	705	A	C4-C5-N7	-5.35	108.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	821	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1262	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1395	A	C4-C5-N7	-5.35	108.02	110.70
26	BA	1496	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1757	A	N9-C4-C5	5.35	107.94	105.80
26	BA	2015	A	C8-N9-C4	5.35	107.94	105.80
26	BA	2792	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	432	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	609	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	1398	A	N9-C4-C5	5.35	107.94	105.80
25	AY	66	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	1815	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	2142	A	N9-C4-C5	5.35	107.94	105.80
26	BA	2654	A	N9-C4-C5	5.35	107.94	105.80
26	BA	2886	A	N9-C4-C5	5.35	107.94	105.80
1	AA	71	A	C4-C5-N7	-5.35	108.03	110.70
1	AA	729	A	C4-C5-N7	-5.35	108.03	110.70
1	AA	747	A	N9-C4-C5	5.35	107.94	105.80
1	AA	1169	A	N9-C4-C5	5.35	107.94	105.80
22	AV	20	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	118	A	C8-N9-C4	5.35	107.94	105.80
26	BA	160	A	C8-N9-C4	5.35	107.94	105.80
26	BA	404	A	N9-C4-C5	5.35	107.94	105.80
26	BA	492	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1433	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	2094	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	2317	A	C8-N9-C4	5.35	107.94	105.80
26	BA	2706	A	N9-C4-C5	5.35	107.94	105.80
26	BA	2826	A	C4-C5-N7	-5.35	108.03	110.70
27	BB	119	A	N9-C4-C5	5.35	107.94	105.80
1	AA	3	A	C8-N9-C4	5.35	107.94	105.80
1	AA	759	A	N9-C4-C5	5.35	107.94	105.80
1	AA	923	A	N9-C4-C5	5.35	107.94	105.80
26	BA	362	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	613	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	654	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	730	A	N9-C4-C5	5.35	107.94	105.80
26	BA	990	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1155	A	N3-C4-N9	5.35	131.68	127.40
26	BA	1453	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1532	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1632	A	C4-C5-N7	-5.35	108.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1672	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	1762	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	1789	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	2764	A	C4-C5-C6	5.35	119.67	117.00
24	AX	21	A	N9-C4-C5	5.35	107.94	105.80
26	BA	655	A	N9-C4-C5	5.35	107.94	105.80
26	BA	819	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	1103	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1156	A	N9-C4-C5	5.35	107.94	105.80
26	BA	1677	A	C4-C5-N7	-5.35	108.03	110.70
26	BA	2679	A	N9-C4-C5	5.35	107.94	105.80
1	AA	704	A	N9-C4-C5	5.34	107.94	105.80
1	AA	815	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1191	A	C4-C5-N7	-5.34	108.03	110.70
25	AY	73	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	300	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	613	A	N9-C4-C5	5.34	107.94	105.80
26	BA	1151	A	N9-C4-C5	5.34	107.94	105.80
26	BA	2541	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	1143	A	N9-C4-C5	5.34	107.94	105.80
26	BA	1553	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	2273	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	2366	A	N9-C4-C5	5.34	107.94	105.80
1	AA	629	A	N9-C4-C5	5.34	107.94	105.80
1	AA	781	A	C4-C5-N7	-5.34	108.03	110.70
25	AY	23	A	N9-C4-C5	5.34	107.94	105.80
26	BA	167	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	191	A	N9-C4-C5	5.34	107.94	105.80
26	BA	632	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	1010	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	1591	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	1977	A	N9-C4-C5	5.34	107.94	105.80
26	BA	2376	A	N9-C4-C5	5.34	107.94	105.80
1	AA	16	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	1306	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1374	A	C4-C5-N7	-5.34	108.03	110.70
25	AY	6	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	83	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	176	A	N9-C4-C5	5.34	107.94	105.80
26	BA	204	A	N3-C4-N9	5.34	131.67	127.40
26	BA	637	A	N9-C4-C5	5.34	107.94	105.80
26	BA	715	A	C4-C5-N7	-5.34	108.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	789	A	N9-C4-C5	5.34	107.94	105.80
26	BA	1262	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	1269	A	N9-C4-C5	5.34	107.94	105.80
26	BA	1548	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	1854	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	2340	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	2868	A	C8-N9-C4	5.34	107.94	105.80
1	AA	189	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1216	A	N9-C4-C5	5.34	107.94	105.80
25	AY	35	A	N9-C4-C5	5.34	107.94	105.80
26	BA	925	A	N9-C4-C5	5.34	107.94	105.80
26	BA	1678	A	N9-C4-C5	5.34	107.94	105.80
26	BA	1866	A	C8-N9-C4	5.34	107.94	105.80
1	AA	210	C	C6-N1-C2	-5.34	118.17	120.30
1	AA	353	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	958	A	C8-N9-C4	5.34	107.93	105.80
1	AA	1163	A	N9-C4-C5	5.34	107.94	105.80
26	BA	1365	A	C8-N9-C4	5.34	107.93	105.80
26	BA	1439	A	C8-N9-C4	5.34	107.94	105.80
26	BA	1477	A	N9-C4-C5	5.34	107.94	105.80
26	BA	1572	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	2054	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	2058	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	2163	A	C4-C5-N7	-5.34	108.03	110.70
26	BA	2792	A	N9-C4-C5	5.34	107.93	105.80
26	BA	2851	A	N9-C4-C5	5.34	107.94	105.80
26	BA	447	A	C4-C5-N7	-5.33	108.03	110.70
26	BA	928	A	N9-C4-C5	5.33	107.93	105.80
26	BA	2587	A	N9-C4-C5	5.33	107.93	105.80
27	BB	109	A	N9-C4-C5	5.33	107.93	105.80
1	AA	1005	A	C8-N9-C4	5.33	107.93	105.80
1	AA	1252	A	C4-C5-N7	-5.33	108.03	110.70
26	BA	1876	A	C4-C5-C6	5.33	119.67	117.00
27	BB	57	A	N9-C4-C5	5.33	107.93	105.80
1	AA	964	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	1082	A	N9-C4-C5	5.33	107.93	105.80
1	AA	1534	A	C8-N9-C4	5.33	107.93	105.80
26	BA	172	A	N9-C4-C5	5.33	107.93	105.80
26	BA	975	A	N9-C4-C5	5.33	107.93	105.80
26	BA	1525	A	C4-C5-N7	-5.33	108.03	110.70
26	BA	2274	A	C4-C5-N7	-5.33	108.03	110.70
26	BA	2386	A	C4-C5-N7	-5.33	108.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2432	A	C4-C5-N7	-5.33	108.03	110.70
26	BA	2835	A	C4-C5-N7	-5.33	108.03	110.70
25	AY	73	A	N9-C4-C5	5.33	107.93	105.80
26	BA	1754	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	181	A	N9-C4-C5	5.33	107.93	105.80
1	AA	559	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	1035	A	N9-C4-C5	5.33	107.93	105.80
26	BA	294	A	C8-N9-C4	5.33	107.93	105.80
26	BA	541	A	N9-C4-C5	5.33	107.93	105.80
26	BA	631	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	282	A	C4-C5-N7	-5.33	108.04	110.70
26	BA	793	A	C4-C5-N7	-5.33	108.04	110.70
26	BA	1077	A	C4-C5-N7	-5.33	108.04	110.70
26	BA	1086	A	C4-C5-N7	-5.33	108.04	110.70
26	BA	1808	A	N9-C4-C5	5.33	107.93	105.80
26	BA	2013	A	C4-C5-N7	-5.33	108.04	110.70
26	BA	2014	A	C4-C5-N7	-5.33	108.04	110.70
26	BA	2052	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	60	A	N9-C4-C5	5.33	107.93	105.80
1	AA	262	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	382	A	N9-C4-C5	5.33	107.93	105.80
1	AA	1191	A	N9-C4-C5	5.33	107.93	105.80
25	AY	41	A	N9-C4-C5	5.33	107.93	105.80
26	BA	345	A	N9-C4-C5	5.33	107.93	105.80
26	BA	503	A	N9-C4-C5	5.33	107.93	105.80
26	BA	1021	A	N9-C4-C5	5.33	107.93	105.80
26	BA	1085	A	N9-C4-C5	5.33	107.93	105.80
26	BA	1477	A	C4-C5-N7	-5.33	108.04	110.70
26	BA	1496	A	C4-C5-N7	-5.33	108.04	110.70
26	BA	1579	A	N9-C4-C5	5.33	107.93	105.80
26	BA	1936	A	C4-C5-N7	-5.33	108.04	110.70
26	BA	2037	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	33	A	N9-C4-C5	5.32	107.93	105.80
1	AA	329	A	C4-C5-N7	-5.32	108.04	110.70
1	AA	523	A	N9-C4-C5	5.32	107.93	105.80
1	AA	1339	A	C8-N9-C4	5.32	107.93	105.80
26	BA	614	A	N9-C4-C5	5.32	107.93	105.80
26	BA	633	A	C8-N9-C4	5.32	107.93	105.80
26	BA	1780	A	N9-C4-C5	5.32	107.93	105.80
26	BA	1919	A	N9-C4-C5	5.32	107.93	105.80
26	BA	2274	A	N9-C4-C5	5.32	107.93	105.80
26	BA	2335	A	C4-C5-N7	-5.32	108.04	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2369	A	N9-C4-C5	5.32	107.93	105.80
26	BA	2412	A	N9-C4-C5	5.32	107.93	105.80
1	AA	459	A	C8-N9-C4	5.32	107.93	105.80
1	AA	1499	A	N9-C4-C5	5.32	107.93	105.80
1	AA	1508	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	342	A	N9-C4-C5	5.32	107.93	105.80
26	BA	457	A	N3-C4-N9	5.32	131.66	127.40
26	BA	1420	A	N9-C4-C5	5.32	107.93	105.80
1	AA	1339	A	N9-C4-C5	5.32	107.93	105.80
26	BA	430	A	C8-N9-C4	5.32	107.93	105.80
26	BA	833	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	1134	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	1244	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	1392	A	C8-N9-C4	5.32	107.93	105.80
26	BA	1717	A	N9-C4-C5	5.32	107.93	105.80
26	BA	1746	A	N9-C4-C5	5.32	107.93	105.80
26	BA	1815	A	N9-C4-C5	5.32	107.93	105.80
27	BB	99	A	C4-C5-N7	-5.32	108.04	110.70
1	AA	238	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	896	A	C8-N9-C4	5.32	107.93	105.80
26	BA	2516	A	N9-C4-C5	5.32	107.93	105.80
26	BA	2835	A	N9-C4-C5	5.32	107.93	105.80
1	AA	640	A	N9-C4-C5	5.32	107.93	105.80
1	AA	1408	A	N9-C4-C5	5.32	107.93	105.80
1	AA	1465	A	C4-C5-N7	-5.32	108.04	110.70
1	AA	1465	A	N9-C4-C5	5.32	107.93	105.80
1	AA	1508	A	N9-C4-C5	5.32	107.93	105.80
23	AW	23	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	1096	A	N9-C4-C5	5.32	107.93	105.80
26	BA	1711	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	2333	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	2565	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	2660	A	N9-C4-C5	5.32	107.93	105.80
26	BA	2700	A	N9-C4-C5	5.32	107.93	105.80
26	BA	449	A	N9-C4-C5	5.32	107.93	105.80
26	BA	586	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	1549	A	C4-C5-N7	-5.32	108.04	110.70
26	BA	2227	A	N9-C4-C5	5.32	107.93	105.80
26	BA	2813	A	C8-N9-C4	5.32	107.93	105.80
27	BB	15	A	N9-C4-C5	5.32	107.93	105.80
1	AA	532	A	C4-C5-N7	-5.31	108.04	110.70
24	AX	76	A	N9-C4-C5	5.31	107.93	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1086	A	C8-N9-C4	5.31	107.93	105.80
26	BA	2211	A	C4-C5-N7	-5.31	108.04	110.70
26	BA	2267	A	C5-C6-N1	5.31	120.36	117.70
1	AA	696	A	C8-N9-C4	5.31	107.92	105.80
24	AX	3	A	N9-C4-C5	5.31	107.92	105.80
26	BA	1029	A	C4-C5-N7	-5.31	108.04	110.70
26	BA	1046	A	C4-C5-N7	-5.31	108.04	110.70
26	BA	1275	A	N9-C4-C5	5.31	107.92	105.80
26	BA	1328	A	N9-C4-C5	5.31	107.92	105.80
26	BA	1490	A	N9-C4-C5	5.31	107.92	105.80
26	BA	1654	A	N9-C4-C5	5.31	107.92	105.80
26	BA	1953	A	C4-C5-N7	-5.31	108.04	110.70
26	BA	1953	A	C8-N9-C4	5.31	107.92	105.80
26	BA	2564	A	C8-N9-C4	5.31	107.92	105.80
26	BA	2757	A	N9-C4-C5	5.31	107.92	105.80
27	BB	45	A	C4-C5-N7	-5.31	108.04	110.70
1	AA	790	A	N9-C4-C5	5.31	107.92	105.80
1	AA	889	A	C4-C5-C6	5.31	119.66	117.00
1	AA	1219	A	C8-N9-C4	5.31	107.92	105.80
25	AY	9	A	C4-C5-N7	-5.31	108.05	110.70
26	BA	173	A	N9-C4-C5	5.31	107.92	105.80
26	BA	920	A	C4-C5-N7	-5.31	108.04	110.70
23	AW	73	A	N9-C4-C5	5.31	107.92	105.80
26	BA	1700	A	N9-C4-C5	5.31	107.92	105.80
26	BA	2765	A	C4-C5-N7	-5.31	108.05	110.70
1	AA	190	A	C4-C5-N7	-5.31	108.05	110.70
1	AA	596	A	N9-C4-C5	5.31	107.92	105.80
1	AA	937	A	N9-C4-C5	5.31	107.92	105.80
1	AA	1254	A	N9-C4-C5	5.31	107.92	105.80
26	BA	204	A	C4-C5-C6	5.31	119.65	117.00
1	AA	196	A	C8-N9-C4	5.31	107.92	105.80
1	AA	523	A	C4-C5-N7	-5.31	108.05	110.70
1	AA	1239	A	N9-C4-C5	5.31	107.92	105.80
1	AA	1319	A	C4-C5-N7	-5.31	108.05	110.70
26	BA	49	A	N9-C4-C5	5.31	107.92	105.80
26	BA	1672	A	N9-C4-C5	5.31	107.92	105.80
23	AW	66	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	299	A	C8-N9-C4	5.30	107.92	105.80
26	BA	654	A	N9-C4-C5	5.30	107.92	105.80
26	BA	1284	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	1698	A	N9-C4-C5	5.30	107.92	105.80
26	BA	1762	A	C8-N9-C4	5.30	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2352	A	N9-C4-C5	5.30	107.92	105.80
26	BA	2425	A	N9-C4-C5	5.30	107.92	105.80
1	AA	1213	A	N9-C4-C5	5.30	107.92	105.80
1	AA	1219	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	1319	A	N9-C4-C5	5.30	107.92	105.80
1	AA	1346	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	222	A	N9-C4-C5	5.30	107.92	105.80
26	BA	556	A	N9-C4-C5	5.30	107.92	105.80
1	AA	2	A	C8-N9-C4	5.30	107.92	105.80
1	AA	238	A	N9-C4-C5	5.30	107.92	105.80
1	AA	279	A	N9-C4-C5	5.30	107.92	105.80
1	AA	414	A	N9-C4-C5	5.30	107.92	105.80
1	AA	959	A	C4-C5-N7	-5.30	108.05	110.70
22	AV	21	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	10	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	547	A	N9-C4-C5	5.30	107.92	105.80
26	BA	981	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	1205	A	N9-C4-C5	5.30	107.92	105.80
26	BA	1262	A	C8-N9-C4	5.30	107.92	105.80
26	BA	1373	A	N9-C4-C5	5.30	107.92	105.80
26	BA	1829	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	81	A	N9-C4-C5	5.30	107.92	105.80
1	AA	306	A	N9-C4-C5	5.30	107.92	105.80
1	AA	754	C	C6-N1-C1'	-5.30	114.44	120.80
1	AA	1257	A	N9-C4-C5	5.30	107.92	105.80
26	BA	513	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	675	A	N9-C4-C5	5.30	107.92	105.80
26	BA	1241	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	1269	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	1393	A	C8-N9-C4	5.30	107.92	105.80
26	BA	1431	A	N9-C4-C5	5.30	107.92	105.80
26	BA	1664	A	C8-N9-C4	5.30	107.92	105.80
26	BA	1938	A	N9-C4-C5	5.30	107.92	105.80
26	BA	2158	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	2407	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	2439	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	50	A	N9-C4-C5	5.30	107.92	105.80
1	AA	1180	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	507	A	N9-C4-C5	5.30	107.92	105.80
26	BA	845	A	C8-N9-C4	5.30	107.92	105.80
26	BA	2020	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	2560	A	C5-C6-N1	5.30	120.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2887	A	N9-C4-C5	5.30	107.92	105.80
1	AA	819	A	N9-C4-C5	5.30	107.92	105.80
1	AA	1014	A	C8-N9-C4	5.30	107.92	105.80
1	AA	1081	A	N9-C4-C5	5.30	107.92	105.80
26	BA	94	A	N9-C4-C5	5.30	107.92	105.80
26	BA	503	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	2088	A	C4-C5-N7	-5.30	108.05	110.70
26	BA	2284	A	N9-C4-C5	5.30	107.92	105.80
26	BA	1583	A	C8-N9-C4	5.29	107.92	105.80
1	AA	746	A	C4-C5-N7	-5.29	108.05	110.70
1	AA	994	A	N9-C4-C5	5.29	107.92	105.80
26	BA	227	A	C4-C5-N7	-5.29	108.05	110.70
26	BA	1080	A	N9-C4-C5	5.29	107.92	105.80
26	BA	1322	A	C4-C5-N7	-5.29	108.05	110.70
26	BA	1635	A	N9-C4-C5	5.29	107.92	105.80
26	BA	1759	A	N9-C4-C5	5.29	107.92	105.80
26	BA	2184	A	C4-C5-N7	-5.29	108.05	110.70
26	BA	2328	A	N9-C4-C5	5.29	107.92	105.80
26	BA	2572	A	N9-C4-C5	5.29	107.92	105.80
1	AA	8	A	N9-C4-C5	5.29	107.92	105.80
1	AA	236	A	C8-N9-C4	5.29	107.92	105.80
1	AA	1021	A	C4-C5-N7	-5.29	108.05	110.70
1	AA	1285	A	N9-C4-C5	5.29	107.92	105.80
1	AA	1318	A	C4-C5-N7	-5.29	108.05	110.70
1	AA	1375	A	N9-C4-C5	5.29	107.92	105.80
22	AV	19	A	C4-C5-N7	-5.29	108.05	110.70
24	AX	23	A	N9-C4-C5	5.29	107.92	105.80
25	AY	38	A	N9-C4-C5	5.29	107.92	105.80
26	BA	332	A	N9-C4-C5	5.29	107.92	105.80
26	BA	631	A	N9-C4-C5	5.29	107.92	105.80
26	BA	761	A	N9-C4-C5	5.29	107.92	105.80
26	BA	800	A	N3-C4-N9	5.29	131.63	127.40
26	BA	2879	A	N9-C4-C5	5.29	107.92	105.80
1	AA	55	A	N9-C4-C5	5.29	107.92	105.80
26	BA	1885	A	N9-C4-C5	5.29	107.92	105.80
1	AA	192	A	C4-C5-N7	-5.29	108.06	110.70
1	AA	607	A	C4-C5-N7	-5.29	108.06	110.70
26	BA	83	A	N9-C4-C5	5.29	107.92	105.80
26	BA	221	A	N9-C4-C5	5.29	107.92	105.80
26	BA	471	A	N9-C4-C5	5.29	107.92	105.80
26	BA	947	A	N9-C4-C5	5.29	107.92	105.80
26	BA	1144	A	N9-C4-C5	5.29	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1711	A	N9-C4-C5	5.29	107.92	105.80
26	BA	2340	A	N9-C4-C5	5.29	107.92	105.80
26	BA	2377	A	N9-C4-C5	5.29	107.92	105.80
1	AA	51	A	N9-C4-C5	5.29	107.91	105.80
1	AA	1130	A	N9-C4-C5	5.29	107.91	105.80
26	BA	586	A	N9-C4-C5	5.29	107.91	105.80
26	BA	1021	A	C4-C5-N7	-5.29	108.06	110.70
26	BA	1354	A	N9-C4-C5	5.29	107.91	105.80
26	BA	2062	A	C8-N9-C4	5.29	107.91	105.80
27	BB	59	A	C4-C5-N7	-5.29	108.06	110.70
1	AA	1167	A	C8-N9-C4	5.28	107.91	105.80
23	AW	31	A	N9-C4-C5	5.28	107.91	105.80
26	BA	52	A	C4-C5-N7	-5.28	108.06	110.70
26	BA	483	A	N9-C4-C5	5.28	107.91	105.80
26	BA	941	A	N9-C4-C5	5.28	107.91	105.80
26	BA	2451	A	C8-N9-C4	5.28	107.91	105.80
27	BB	50	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	270	A	C4-C5-N7	-5.28	108.06	110.70
26	BA	21	A	N9-C4-C5	5.28	107.91	105.80
26	BA	282	A	N9-C4-C5	5.28	107.91	105.80
26	BA	368	A	N9-C4-C5	5.28	107.91	105.80
26	BA	2518	A	N9-C4-C5	5.28	107.91	105.80
1	AA	161	A	N9-C4-C5	5.28	107.91	105.80
1	AA	675	A	N9-C4-C5	5.28	107.91	105.80
1	AA	1483	A	N9-C4-C5	5.28	107.91	105.80
1	AA	1518	A	N9-C4-C5	5.28	107.91	105.80
26	BA	218	A	N9-C4-C5	5.28	107.91	105.80
26	BA	643	A	N9-C4-C5	5.28	107.91	105.80
26	BA	1570	A	C4-C5-N7	-5.28	108.06	110.70
26	BA	1572	A	N9-C4-C5	5.28	107.91	105.80
26	BA	2171	A	C4-C5-N7	-5.28	108.06	110.70
26	BA	2450	A	C8-N9-C4	5.28	107.91	105.80
26	BA	2749	A	N9-C4-C5	5.28	107.91	105.80
1	AA	996	A	N9-C4-C5	5.28	107.91	105.80
26	BA	1785	A	N3-C4-N9	5.28	131.62	127.40
26	BA	2082	A	N9-C4-C5	5.28	107.91	105.80
26	BA	2095	A	N9-C4-C5	5.28	107.91	105.80
1	AA	430	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	864	A	N9-C4-C5	5.28	107.91	105.80
1	AA	1261	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	1500	A	N9-C4-C5	5.28	107.91	105.80
22	AV	15	A	N9-C4-C5	5.28	107.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	255	A	C4-C5-N7	-5.28	108.06	110.70
26	BA	1090	A	N9-C4-C5	5.28	107.91	105.80
26	BA	1284	A	N9-C4-C5	5.28	107.91	105.80
26	BA	2476	A	N9-C4-C5	5.28	107.91	105.80
1	AA	496	A	C4-C5-N7	-5.28	108.06	110.70
26	BA	152	A	N9-C4-C5	5.28	107.91	105.80
26	BA	497	A	N9-C4-C5	5.28	107.91	105.80
26	BA	1010	A	C8-N9-C4	5.28	107.91	105.80
26	BA	1096	A	C4-C5-N7	-5.28	108.06	110.70
26	BA	1981	A	C8-N9-C4	5.28	107.91	105.80
26	BA	2191	A	C4-C5-N7	-5.28	108.06	110.70
26	BA	1387	A	C4-C5-N7	-5.27	108.06	110.70
1	AA	1005	A	C4-C5-N7	-5.27	108.06	110.70
26	BA	412	A	N9-C4-C5	5.27	107.91	105.80
26	BA	2432	A	N9-C4-C5	5.27	107.91	105.80
1	AA	356	A	C4-C5-N7	-5.27	108.06	110.70
26	BA	1549	A	N9-C4-C5	5.27	107.91	105.80
1	AA	192	A	N9-C4-C5	5.27	107.91	105.80
1	AA	609	A	N9-C4-C5	5.27	107.91	105.80
1	AA	1101	A	N9-C4-C5	5.27	107.91	105.80
26	BA	1583	A	C4-C5-N7	-5.27	108.06	110.70
26	BA	2531	A	C4-C5-N7	-5.27	108.06	110.70
1	AA	1396	A	N9-C4-C5	5.27	107.91	105.80
25	AY	33	U	C2-N1-C1'	5.27	124.02	117.70
26	BA	256	A	N9-C4-C5	5.27	107.91	105.80
26	BA	644	A	C4-C5-N7	-5.27	108.07	110.70
26	BA	1901	A	C5-C6-N1	5.27	120.33	117.70
26	BA	2184	A	N9-C4-C5	5.27	107.91	105.80
26	BA	2765	A	N9-C4-C5	5.27	107.91	105.80
1	AA	98	A	C4-C5-N7	-5.27	108.07	110.70
1	AA	1016	A	C8-N9-C4	5.26	107.91	105.80
1	AA	1201	A	N9-C4-C5	5.26	107.91	105.80
26	BA	503	A	C5-C6-N1	5.26	120.33	117.70
26	BA	1791	A	C8-N9-C4	5.26	107.91	105.80
26	BA	2097	A	C4-C5-N7	-5.26	108.07	110.70
26	BA	2541	A	N9-C4-C5	5.26	107.91	105.80
1	AA	1324	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	964	A	N9-C4-C5	5.26	107.90	105.80
1	AA	1363	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	1502	A	N9-C4-C5	5.26	107.90	105.80
26	BA	10	A	N9-C4-C5	5.26	107.91	105.80
26	BA	599	A	C5-C6-N1	5.26	120.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	2358	A	N9-C4-C5	5.26	107.91	105.80
26	BA	2426	A	N9-C4-C5	5.26	107.91	105.80
26	BA	2461	A	N9-C4-C5	5.26	107.91	105.80
26	BA	2547	A	C4-C5-N7	-5.26	108.07	110.70
26	BA	2856	A	N9-C4-C5	5.26	107.91	105.80
1	AA	746	A	N9-C4-C5	5.26	107.90	105.80
1	AA	938	A	N9-C4-C5	5.26	107.90	105.80
26	BA	1522	A	C4-C5-N7	-5.26	108.07	110.70
26	BA	1787	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	432	A	N9-C4-C5	5.26	107.90	105.80
23	AW	66	A	N9-C4-C5	5.26	107.90	105.80
26	BA	196	A	C8-N9-C4	5.26	107.90	105.80
26	BA	1434	A	N9-C4-C5	5.26	107.90	105.80
26	BA	1745	A	C4-C5-N7	-5.26	108.07	110.70
26	BA	2080	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	559	A	N9-C4-C5	5.26	107.90	105.80
26	BA	2014	A	N9-C4-C5	5.26	107.90	105.80
26	BA	2451	A	C4-C5-C6	5.26	119.63	117.00
1	AA	1362	A	C4-C5-N7	-5.25	108.07	110.70
26	BA	52	A	N9-C4-C5	5.25	107.90	105.80
26	BA	2328	A	C4-C5-N7	-5.25	108.07	110.70
27	BB	73	A	C4-C5-N7	-5.25	108.07	110.70
26	BA	609	A	N9-C4-C5	5.25	107.90	105.80
26	BA	1048	A	N9-C4-C5	5.25	107.90	105.80
26	BA	2468	A	N9-C4-C5	5.25	107.90	105.80
27	BB	39	A	N9-C4-C5	5.25	107.90	105.80
1	AA	74	A	C8-N9-C4	5.25	107.90	105.80
1	AA	547	A	N9-C4-C5	5.25	107.90	105.80
1	AA	1507	A	C4-C5-N7	-5.25	108.07	110.70
26	BA	582	A	C4-C5-N7	-5.25	108.07	110.70
26	BA	743	A	C4-C5-N7	-5.25	108.07	110.70
26	BA	1591	A	N9-C4-C5	5.25	107.90	105.80
26	BA	2826	A	N9-C4-C5	5.25	107.90	105.80
26	BA	2860	A	C4-C5-N7	-5.25	108.08	110.70
26	BA	2602	A	N9-C4-C5	5.25	107.90	105.80
1	AA	250	A	N9-C4-C5	5.25	107.90	105.80
1	AA	621	A	N9-C4-C5	5.25	107.90	105.80
26	BA	146	A	N9-C4-C5	5.25	107.90	105.80
26	BA	482	A	N9-C4-C5	5.25	107.90	105.80
26	BA	1088	A	N9-C4-C5	5.25	107.90	105.80
1	AA	389	A	N9-C4-C5	5.25	107.90	105.80
1	AA	496	A	N9-C4-C5	5.25	107.90	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	603	A	N9-C4-C5	5.25	107.90	105.80
26	BA	782	A	C4-C5-N7	-5.25	108.08	110.70
26	BA	917	A	N9-C4-C5	5.25	107.90	105.80
26	BA	1008	A	N9-C4-C5	5.25	107.90	105.80
26	BA	1470	A	N9-C4-C5	5.25	107.90	105.80
26	BA	1535	A	N9-C4-C5	5.25	107.90	105.80
1	AA	901	A	C4-C5-N7	-5.25	108.08	110.70
1	AA	174	A	N9-C4-C5	5.24	107.90	105.80
1	AA	452	A	N3-C4-N9	5.24	131.59	127.40
1	AA	864	A	C4-C5-N7	-5.24	108.08	110.70
26	BA	457	A	C4-C5-C6	5.24	119.62	117.00
26	BA	2037	A	N9-C4-C5	5.24	107.90	105.80
27	BB	66	A	N9-C4-C5	5.24	107.90	105.80
26	BA	1490	A	C8-N9-C4	5.24	107.90	105.80
1	AA	478	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	1324	A	N9-C4-C5	5.24	107.90	105.80
26	BA	415	A	N9-C4-C5	5.24	107.90	105.80
26	BA	572	A	C4-C5-N7	-5.24	108.08	110.70
26	BA	984	A	C8-N9-C4	5.24	107.90	105.80
26	BA	1801	A	N9-C4-C5	5.24	107.90	105.80
26	BA	1928	A	C8-N9-C4	5.24	107.90	105.80
26	BA	2097	A	N9-C4-C5	5.24	107.90	105.80
26	BA	2560	A	C4-C5-N7	-5.24	108.08	110.70
26	BA	272	A	N9-C4-C5	5.24	107.89	105.80
26	BA	402	A	N9-C4-C5	5.24	107.89	105.80
26	BA	1265	A	N9-C4-C5	5.24	107.90	105.80
26	BA	1535	A	C8-N9-C4	5.24	107.89	105.80
26	BA	1791	A	C4-C5-N7	-5.24	108.08	110.70
26	BA	2328	A	C8-N9-C4	5.24	107.89	105.80
26	BA	197	A	N9-C4-C5	5.24	107.89	105.80
26	BA	1084	A	C8-N9-C4	5.24	107.89	105.80
26	BA	1253	A	N9-C4-C5	5.24	107.89	105.80
26	BA	1936	A	N9-C4-C5	5.24	107.89	105.80
22	AV	20	A	N9-C4-C5	5.24	107.89	105.80
24	AX	24	A	C4-C5-N7	-5.24	108.08	110.70
26	BA	142	A	C5-C6-N1	5.24	120.32	117.70
26	BA	1322	A	N9-C4-C5	5.24	107.89	105.80
26	BA	1548	A	N9-C4-C5	5.24	107.89	105.80
26	BA	2893	A	N9-C4-C5	5.24	107.89	105.80
1	AA	1346	A	N9-C4-C5	5.23	107.89	105.80
1	AA	546	A	N9-C4-C5	5.23	107.89	105.80
26	BA	430	A	N9-C4-C5	5.23	107.89	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1321	A	N9-C4-C5	5.23	107.89	105.80
1	AA	451	A	C4-C5-N7	-5.23	108.08	110.70
1	AA	1022	A	C4-C5-N7	-5.23	108.08	110.70
26	BA	251	A	C4-C5-N7	-5.23	108.08	110.70
26	BA	279	A	N9-C4-C5	5.23	107.89	105.80
26	BA	1722	A	N9-C4-C5	5.23	107.89	105.80
1	AA	1102	A	C4-C5-N7	-5.23	108.09	110.70
1	AA	373	A	N9-C4-C5	5.23	107.89	105.80
1	AA	532	A	N9-C4-C5	5.23	107.89	105.80
1	AA	923	A	C4-C5-N7	-5.23	108.09	110.70
26	BA	794	A	N9-C4-C5	5.23	107.89	105.80
26	BA	2407	A	N9-C4-C5	5.23	107.89	105.80
26	BA	2725	A	C4-C5-N7	-5.23	108.09	110.70
1	AA	389	A	C4-C5-N7	-5.22	108.09	110.70
26	BA	142	A	N9-C4-C5	5.22	107.89	105.80
26	BA	362	A	N9-C4-C5	5.22	107.89	105.80
26	BA	2273	A	N9-C4-C5	5.22	107.89	105.80
1	AA	935	A	N9-C4-C5	5.22	107.89	105.80
1	AA	977	A	N9-C4-C5	5.22	107.89	105.80
26	BA	1614	A	N9-C4-C5	5.22	107.89	105.80
26	BA	1655	A	N9-C4-C5	5.22	107.89	105.80
26	BA	2117	A	N9-C4-C5	5.22	107.89	105.80
26	BA	2378	A	C8-N9-C4	5.22	107.89	105.80
26	BA	2757	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	1329	A	C4-C5-C6	5.22	119.61	117.00
26	BA	1077	A	N9-C4-C5	5.22	107.89	105.80
26	BA	1359	A	C4-C5-N7	-5.22	108.09	110.70
25	AY	26	A	N9-C4-C5	5.22	107.89	105.80
26	BA	63	A	C4-C5-N7	-5.22	108.09	110.70
26	BA	514	A	C8-N9-C4	5.22	107.89	105.80
26	BA	979	A	N9-C4-C5	5.22	107.89	105.80
26	BA	2336	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	321	A	N9-C4-C5	5.22	107.89	105.80
1	AA	1021	A	N9-C4-C5	5.22	107.89	105.80
26	BA	73	A	C8-N9-C4	5.22	107.89	105.80
26	BA	91	A	C4-C5-N7	-5.22	108.09	110.70
26	BA	1713	A	N9-C4-C5	5.22	107.89	105.80
1	AA	814	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	1167	A	C4-C5-N7	-5.22	108.09	110.70
26	BA	384	A	C8-N9-C4	5.22	107.89	105.80
26	BA	920	A	N9-C4-C5	5.22	107.89	105.80
26	BA	1810	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	977	A	C4-C5-N7	-5.21	108.09	110.70
1	AA	1236	A	N9-C4-C5	5.21	107.89	105.80
26	BA	1276	A	C4-C5-N7	-5.21	108.09	110.70
26	BA	1785	A	C4-C5-C6	5.21	119.61	117.00
26	BA	2051	A	C8-N9-C4	5.21	107.89	105.80
26	BA	2163	A	N9-C4-C5	5.21	107.89	105.80
1	AA	959	A	C8-N9-C4	5.21	107.89	105.80
26	BA	752	A	N9-C4-C5	5.21	107.89	105.80
26	BA	1677	A	N9-C4-C5	5.21	107.89	105.80
26	BA	2033	A	N3-C4-N9	5.21	131.57	127.40
1	AA	482	A	C4-C5-N7	-5.21	108.09	110.70
26	BA	2094	A	N9-C4-C5	5.21	107.88	105.80
26	BA	2469	A	C4-C5-C6	5.21	119.61	117.00
1	AA	499	A	N3-C4-N9	5.21	131.57	127.40
1	AA	1362	A	N9-C4-C5	5.21	107.88	105.80
26	BA	1327	A	N9-C4-C5	5.21	107.88	105.80
1	AA	495	A	C5-C6-N1	5.21	120.30	117.70
1	AA	510	A	C8-N9-C4	5.21	107.88	105.80
26	BA	196	A	C4-C5-N7	-5.21	108.10	110.70
26	BA	528	A	C4-C5-N7	-5.21	108.09	110.70
26	BA	820	A	N9-C4-C5	5.21	107.88	105.80
1	AA	356	A	N9-C4-C5	5.21	107.88	105.80
26	BA	415	A	C4-C5-N7	-5.21	108.10	110.70
26	BA	582	A	N9-C4-C5	5.21	107.88	105.80
26	BA	2062	A	N9-C4-C5	5.21	107.88	105.80
1	AA	109	A	N9-C4-C5	5.20	107.88	105.80
1	AA	975	A	N9-C4-C5	5.20	107.88	105.80
1	AA	1357	A	C4-C5-N7	-5.20	108.10	110.70
26	BA	53	A	C8-N9-C4	5.20	107.88	105.80
26	BA	391	A	N9-C4-C5	5.20	107.88	105.80
26	BA	1809	A	C8-N9-C4	5.20	107.88	105.80
26	BA	2054	A	N9-C4-C5	5.20	107.88	105.80
26	BA	2080	A	N9-C4-C5	5.20	107.88	105.80
1	AA	1152	A	C4-C5-N7	-5.20	108.10	110.70
1	AA	572	A	C8-N9-C4	5.20	107.88	105.80
26	BA	103	A	N9-C4-C5	5.20	107.88	105.80
26	BA	1134	A	N9-C4-C5	5.20	107.88	105.80
1	AA	923	A	C8-N9-C4	5.20	107.88	105.80
1	AA	983	A	C5-C6-N1	5.20	120.30	117.70
1	AA	983	A	N9-C4-C5	5.20	107.88	105.80
26	BA	2598	A	C4-C5-N7	-5.20	108.10	110.70
26	BA	1378	A	C5-C6-N1	5.20	120.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1603	A	C4-C5-N7	-5.20	108.10	110.70
26	BA	2392	A	C8-N9-C4	5.20	107.88	105.80
1	AA	1299	A	N9-C4-C5	5.20	107.88	105.80
26	BA	616	A	N9-C4-C5	5.20	107.88	105.80
26	BA	1872	A	C8-N9-C4	5.19	107.88	105.80
26	BA	1970	A	N9-C4-C5	5.19	107.88	105.80
1	AA	16	A	N9-C4-C5	5.19	107.88	105.80
1	AA	435	A	C5-C6-N1	5.19	120.30	117.70
1	AA	872	A	C8-N9-C4	5.19	107.88	105.80
1	AA	1394	A	N9-C4-C5	5.19	107.88	105.80
26	BA	1754	A	N9-C4-C5	5.19	107.88	105.80
26	BA	1866	A	N9-C4-C5	5.19	107.88	105.80
26	BA	1901	A	C8-N9-C4	5.19	107.88	105.80
26	BA	2013	A	N9-C4-C5	5.19	107.88	105.80
26	BA	2439	A	N9-C4-C5	5.19	107.88	105.80
26	BA	73	A	C4-C5-N7	-5.19	108.11	110.70
1	AA	270	A	N9-C4-C5	5.19	107.88	105.80
1	AA	1261	A	N9-C4-C5	5.19	107.88	105.80
26	BA	752	A	C4-C5-N7	-5.19	108.11	110.70
26	BA	833	A	C8-N9-C4	5.19	107.88	105.80
26	BA	960	A	C4-C5-N7	-5.19	108.11	110.70
26	BA	2114	A	C5-C6-N1	5.19	120.29	117.70
26	BA	2776	A	N9-C4-C5	5.19	107.88	105.80
1	AA	32	A	N9-C4-C5	5.19	107.87	105.80
26	BA	447	A	N9-C4-C5	5.19	107.88	105.80
26	BA	1504	A	N9-C4-C5	5.19	107.87	105.80
26	BA	1603	A	N9-C4-C5	5.19	107.87	105.80
26	BA	677	A	N9-C4-C5	5.18	107.87	105.80
26	BA	2665	A	N9-C4-C5	5.18	107.87	105.80
1	AA	162	A	N9-C4-C5	5.18	107.87	105.80
23	AW	26	A	C5-C6-N1	5.18	120.29	117.70
26	BA	793	A	N9-C4-C5	5.18	107.87	105.80
26	BA	1244	A	N9-C4-C5	5.18	107.87	105.80
26	BA	1583	A	N9-C4-C5	5.18	107.87	105.80
1	AA	478	A	N9-C4-C5	5.18	107.87	105.80
25	AY	6	A	N9-C4-C5	5.18	107.87	105.80
25	AY	9	A	N9-C4-C5	5.18	107.87	105.80
26	BA	196	A	N9-C4-C5	5.18	107.87	105.80
26	BA	1876	A	C5-C6-N1	5.18	120.29	117.70
26	BA	2054	A	C5-C6-N1	5.18	120.29	117.70
26	BA	2297	A	C4-C5-N7	-5.18	108.11	110.70
1	AA	1429	A	N9-C4-C5	5.18	107.87	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	1387	A	N9-C4-C5	5.18	107.87	105.80
26	BA	1634	A	N9-C4-C5	5.18	107.87	105.80
26	BA	1664	A	C4-C5-N7	-5.18	108.11	110.70
26	BA	190	A	N9-C4-C5	5.18	107.87	105.80
26	BA	2169	A	C4-C5-N7	-5.18	108.11	110.70
26	BA	2267	A	C4-C5-N7	-5.18	108.11	110.70
26	BA	2451	A	C5-C6-N1	5.18	120.29	117.70
26	BA	689	A	C4-C5-N7	-5.17	108.11	110.70
26	BA	743	A	N9-C4-C5	5.17	107.87	105.80
26	BA	1070	A	N9-C4-C5	5.17	107.87	105.80
26	BA	1614	A	C4-C5-N7	-5.17	108.11	110.70
26	BA	2088	A	N9-C4-C5	5.17	107.87	105.80
1	AA	300	A	N9-C4-C5	5.17	107.87	105.80
1	AA	1350	A	C4-C5-N7	-5.17	108.11	110.70
26	BA	706	A	N9-C4-C5	5.17	107.87	105.80
26	BA	1395	A	N9-C4-C5	5.17	107.87	105.80
26	BA	2327	A	C8-N9-C4	5.17	107.87	105.80
1	AA	983	A	C4-C5-N7	-5.17	108.11	110.70
26	BA	1570	A	N9-C4-C5	5.17	107.87	105.80
1	AA	74	A	N3-C4-N9	5.17	131.53	127.40
1	AA	98	A	N9-C4-C5	5.17	107.87	105.80
1	AA	432	A	C5-C6-N1	5.17	120.28	117.70
1	AA	908	A	N9-C4-C5	5.17	107.87	105.80
26	BA	479	A	N9-C4-C5	5.17	107.87	105.80
26	BA	2191	A	N9-C4-C5	5.17	107.87	105.80
1	AA	1102	A	C5-C6-N1	5.17	120.28	117.70
25	AY	66	A	N9-C4-C5	5.17	107.87	105.80
26	BA	505	A	N9-C4-C5	5.17	107.87	105.80
26	BA	1745	A	N9-C4-C5	5.17	107.87	105.80
26	BA	1899	A	C4-C5-N7	-5.17	108.12	110.70
22	AV	19	A	N9-C4-C5	5.16	107.86	105.80
1	AA	728	A	C8-N9-C4	5.16	107.86	105.80
26	BA	1046	A	N9-C4-C5	5.16	107.86	105.80
26	BA	2459	A	C5-C6-N1	5.16	120.28	117.70
1	AA	781	A	N9-C4-C5	5.16	107.86	105.80
1	AA	1357	A	N9-C4-C5	5.16	107.86	105.80
24	AX	24	A	N9-C4-C5	5.16	107.86	105.80
26	BA	2287	A	C8-N9-C4	5.16	107.86	105.80
26	BA	74	A	N9-C4-C5	5.16	107.86	105.80
26	BA	1969	A	N9-C4-C5	5.16	107.86	105.80
1	AA	431	A	C8-N9-C4	5.16	107.86	105.80
26	BA	845	A	C4-C5-N7	-5.16	108.12	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	607	A	N9-C4-C5	5.16	107.86	105.80
1	AA	968	A	N9-C4-C5	5.16	107.86	105.80
26	BA	750	A	C4-C5-N7	-5.16	108.12	110.70
27	BB	73	A	N9-C4-C5	5.16	107.86	105.80
1	AA	1318	A	N9-C4-C5	5.15	107.86	105.80
27	BB	50	A	N9-C4-C5	5.15	107.86	105.80
1	AA	353	A	N9-C4-C5	5.15	107.86	105.80
1	AA	1418	A	C8-N9-C4	5.15	107.86	105.80
1	AA	487	A	N9-C4-C5	5.15	107.86	105.80
26	BA	430	A	C4-C5-N7	-5.15	108.12	110.70
26	BA	685	A	C4-C5-N7	-5.15	108.12	110.70
26	BA	2820	A	C8-N9-C4	5.15	107.86	105.80
1	AA	873	A	N9-C4-C5	5.15	107.86	105.80
26	BA	131	A	C5-C6-N1	5.15	120.28	117.70
26	BA	52	A	C8-N9-C4	5.15	107.86	105.80
26	BA	119	A	N3-C4-N9	5.15	131.52	127.40
26	BA	1214	A	C5-C6-N1	5.15	120.27	117.70
26	BA	1226	A	C8-N9-C4	5.15	107.86	105.80
26	BA	1676	A	C4-C5-N7	-5.15	108.13	110.70
26	BA	2077	A	C4-C5-N7	-5.15	108.13	110.70
1	AA	977	A	C8-N9-C4	5.15	107.86	105.80
1	AA	55	A	C5-C6-N1	5.14	120.27	117.70
1	AA	563	A	C8-N9-C4	5.14	107.86	105.80
26	BA	1241	A	N9-C4-C5	5.14	107.86	105.80
26	BA	2058	A	C8-N9-C4	5.14	107.86	105.80
26	BA	2267	A	N9-C4-C5	5.14	107.86	105.80
26	BA	119	A	C5-C6-N1	5.14	120.27	117.70
26	BA	782	A	N9-C4-C5	5.14	107.86	105.80
26	BA	1787	A	N9-C4-C5	5.14	107.86	105.80
26	BA	1810	A	N9-C4-C5	5.14	107.86	105.80
26	BA	2662	A	C8-N9-C4	5.14	107.86	105.80
27	BB	45	A	N9-C4-C5	5.14	107.86	105.80
1	AA	452	A	C4-C5-C6	5.14	119.57	117.00
1	AA	865	A	C4-C5-N7	-5.14	108.13	110.70
22	AV	21	A	N9-C4-C5	5.14	107.86	105.80
1	AA	482	A	N9-C4-C5	5.14	107.86	105.80
26	BA	63	A	N9-C4-C5	5.14	107.86	105.80
26	BA	231	A	C5-C6-N1	5.14	120.27	117.70
1	AA	397	A	C8-N9-C4	5.14	107.85	105.80
26	BA	1676	A	N9-C4-C5	5.14	107.86	105.80
1	AA	1157	A	C4-C5-N7	-5.13	108.13	110.70
1	AA	1044	A	C4-C5-N7	-5.13	108.13	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	644	A	C5-C6-N1	5.13	120.27	117.70
26	BA	2333	A	N9-C4-C5	5.13	107.85	105.80
26	BA	2766	A	C4-C5-N7	-5.13	108.13	110.70
26	BA	384	A	C4-C5-N7	-5.13	108.13	110.70
26	BA	401	A	N9-C4-C5	5.13	107.85	105.80
26	BA	2531	A	N9-C4-C5	5.13	107.85	105.80
1	AA	865	A	N9-C4-C5	5.13	107.85	105.80
23	AW	23	A	N9-C4-C5	5.13	107.85	105.80
26	BA	2823	A	C4-C5-N7	-5.13	108.14	110.70
1	AA	451	A	N9-C4-C5	5.13	107.85	105.80
1	AA	622	A	C4-C5-C6	5.13	119.56	117.00
1	AA	1080	A	C8-N9-C4	5.13	107.85	105.80
26	BA	1664	A	C5-C6-N1	5.13	120.26	117.70
26	BA	1784	A	N9-C4-C5	5.13	107.85	105.80
26	BA	330	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	907	A	N9-C4-C5	5.12	107.85	105.80
1	AA	1332	A	C8-N9-C4	5.12	107.85	105.80
26	BA	845	A	N9-C4-C5	5.12	107.85	105.80
26	BA	2799	A	C4-C5-N7	-5.12	108.14	110.70
26	BA	572	A	C5-C6-N1	5.12	120.26	117.70
26	BA	2725	A	N9-C4-C5	5.12	107.85	105.80
26	BA	2778	A	N9-C4-C5	5.12	107.85	105.80
26	BA	863	A	C4-C5-N7	-5.12	108.14	110.70
26	BA	2336	A	N9-C4-C5	5.12	107.85	105.80
26	BA	909	A	C5-C6-N1	5.11	120.26	117.70
26	BA	1900	A	N9-C4-C5	5.11	107.84	105.80
26	BA	2471	A	C5-C6-N1	5.11	120.26	117.70
26	BA	783	A	C5-C6-N1	5.11	120.25	117.70
26	BA	783	A	C8-N9-C4	5.11	107.84	105.80
26	BA	1669	A	C5-C6-N1	5.11	120.25	117.70
1	AA	1350	A	C5-C6-N1	5.11	120.25	117.70
24	AX	19	U	C4-C5-C6	-5.11	116.64	119.70
26	BA	127	A	C8-N9-C4	5.11	107.84	105.80
26	BA	532	A	C8-N9-C4	5.11	107.84	105.80
26	BA	1276	A	C5-C6-N1	5.11	120.25	117.70
26	BA	2800	A	C5-C6-N1	5.11	120.25	117.70
26	BA	255	A	N9-C4-C5	5.11	107.84	105.80
26	BA	1664	A	N9-C4-C5	5.11	107.84	105.80
26	BA	2765	A	C8-N9-C4	5.11	107.84	105.80
26	BA	532	A	C4-C5-N7	-5.10	108.15	110.70
26	BA	330	A	C5-C6-N1	5.10	120.25	117.70
26	BA	466	A	C4-C5-N7	-5.10	108.15	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BB	29	A	C8-N9-C4	5.10	107.84	105.80
27	BB	59	A	N9-C4-C5	5.10	107.84	105.80
1	AA	608	A	C5-C6-N1	5.10	120.25	117.70
26	BA	53	A	C5-C6-N1	5.10	120.25	117.70
26	BA	2311	A	N9-C4-C5	5.10	107.84	105.80
1	AA	1507	A	N9-C4-C5	5.10	107.84	105.80
26	BA	689	A	N9-C4-C5	5.10	107.84	105.80
26	BA	2158	A	N9-C4-C5	5.10	107.84	105.80
26	BA	470	A	N9-C4-C5	5.09	107.84	105.80
26	BA	572	A	N9-C4-C5	5.09	107.84	105.80
26	BA	1553	A	N9-C4-C5	5.09	107.84	105.80
26	BA	1829	A	N9-C4-C5	5.09	107.84	105.80
26	BA	2297	A	N9-C4-C5	5.09	107.84	105.80
26	BA	2469	A	C5-C6-N1	5.09	120.25	117.70
1	AA	1022	A	N9-C4-C5	5.09	107.84	105.80
26	BA	2287	A	C5-C6-N1	5.09	120.25	117.70
26	BA	2070	A	C5-C6-N1	5.09	120.24	117.70
26	BA	933	A	C4-C5-N7	-5.09	108.16	110.70
24	AX	20	U	C4-C5-C6	-5.08	116.65	119.70
26	BA	1669	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	546	A	C4-C5-N7	-5.08	108.16	110.70
26	BA	1276	A	N9-C4-C5	5.08	107.83	105.80
26	BA	2171	A	N9-C4-C5	5.08	107.83	105.80
26	BA	2461	A	C5-C6-N1	5.08	120.24	117.70
1	AA	706	A	C5-C6-N1	5.08	120.24	117.70
26	BA	1522	A	C5-C6-N1	5.08	120.24	117.70
1	AA	563	A	C4-C5-N7	-5.08	108.16	110.70
23	AW	23	A	C5-C6-N1	5.08	120.24	117.70
26	BA	2675	A	C4-C5-N7	-5.08	108.16	110.70
26	BA	2823	A	N9-C4-C5	5.08	107.83	105.80
1	AA	1493	A	C8-N9-C4	5.08	107.83	105.80
1	AA	412	A	C5-C6-N1	5.08	120.24	117.70
26	BA	449	A	C5-C6-N1	5.08	120.24	117.70
26	BA	1029	A	N9-C4-C5	5.07	107.83	105.80
26	BA	1213	A	N9-C4-C5	5.07	107.83	105.80
1	AA	766	A	C5-C6-N1	5.07	120.23	117.70
1	AA	1468	A	N9-C4-C5	5.07	107.83	105.80
26	BA	91	A	N9-C4-C5	5.07	107.83	105.80
26	BA	2800	A	C4-C5-N7	-5.07	108.17	110.70
1	AA	495	A	C4-C5-N7	-5.07	108.17	110.70
1	AA	1044	A	C5-C6-N1	5.07	120.23	117.70
1	AA	1167	A	N9-C4-C5	5.07	107.83	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BA	384	A	N9-C4-C5	5.07	107.83	105.80
23	AW	20	U	C4-C5-C6	-5.07	116.66	119.70
26	BA	142	A	C4-C5-N7	-5.07	108.17	110.70
26	BA	2287	A	C4-C5-N7	-5.07	108.17	110.70
26	BA	2430	A	C4-C5-N7	-5.07	108.17	110.70
1	AA	1333	A	C5-C6-N1	5.06	120.23	117.70
24	AX	16	U	C4-C5-C6	-5.06	116.66	119.70
1	AA	478	A	C5-C6-N1	5.06	120.23	117.70
1	AA	546	A	C8-N9-C4	5.06	107.83	105.80
1	AA	1350	A	N9-C4-C5	5.06	107.83	105.80
26	BA	1876	A	C8-N9-C4	5.06	107.83	105.80
26	BA	2547	A	N9-C4-C5	5.06	107.83	105.80
26	BA	2169	A	N9-C4-C5	5.06	107.82	105.80
24	AX	24	A	C5-C6-N1	5.06	120.23	117.70
26	BA	633	A	C4-C5-N7	-5.06	108.17	110.70
26	BA	2459	A	C4-C5-N7	-5.06	108.17	110.70
1	AA	171	A	C5-C6-N1	5.06	120.23	117.70
1	AA	1363	A	N9-C4-C5	5.06	107.82	105.80
26	BA	371	A	C5-C6-N1	5.06	120.23	117.70
26	BA	2077	A	C5-C6-N1	5.06	120.23	117.70
26	BA	2211	A	N9-C4-C5	5.05	107.82	105.80
26	BA	1899	A	C5-C6-N1	5.05	120.23	117.70
1	AA	190	A	N9-C4-C5	5.05	107.82	105.80
1	AA	1329	A	N3-C4-N9	5.05	131.44	127.40
26	BA	644	A	N9-C4-C5	5.05	107.82	105.80
26	BA	2114	A	C4-C5-N7	-5.05	108.18	110.70
26	BA	2725	A	C5-C6-N1	5.05	120.22	117.70
1	AA	1299	A	C5-C6-N1	5.05	120.22	117.70
26	BA	685	A	N9-C4-C5	5.05	107.82	105.80
26	BA	2748	A	N9-C4-C5	5.05	107.82	105.80
26	BA	689	A	C5-C6-N1	5.04	120.22	117.70
26	BA	227	A	N9-C4-C5	5.04	107.82	105.80
26	BA	750	A	C5-C6-N1	5.04	120.22	117.70
26	BA	2516	A	C5-C6-N1	5.04	120.22	117.70
27	BB	78	A	C5-C6-N1	5.04	120.22	117.70
26	BA	1494	A	C5-C6-N1	5.04	120.22	117.70
26	BA	933	A	C5-C6-N1	5.04	120.22	117.70
1	AA	539	A	C5-C6-N1	5.04	120.22	117.70
1	AA	1152	A	N9-C4-C5	5.04	107.81	105.80
26	BA	546	U	C6-N1-C1'	-5.04	114.15	121.20
26	BA	1378	A	N3-C4-N9	5.04	131.43	127.40
26	BA	2459	A	N9-C4-C5	5.04	107.81	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	26	A	C5-C6-N1	5.03	120.22	117.70
26	BA	632	A	C8-N9-C4	5.03	107.81	105.80
26	BA	705	A	N9-C4-C5	5.03	107.81	105.80
1	AA	1252	A	C8-N9-C4	5.03	107.81	105.80
26	BA	1783	A	C8-N9-C4	5.03	107.81	105.80
1	AA	116	A	C8-N9-C4	5.03	107.81	105.80
26	BA	1669	A	N9-C4-C5	5.03	107.81	105.80
1	AA	1157	A	C5-C6-N1	5.02	120.21	117.70
26	BA	142	A	C8-N9-C4	5.02	107.81	105.80
26	BA	2267	A	C8-N9-C4	5.02	107.81	105.80
26	BA	2662	A	N9-C4-C5	5.02	107.81	105.80
26	BA	2765	A	C5-C6-N1	5.02	120.21	117.70
1	AA	356	A	C5-C6-N1	5.02	120.21	117.70
26	BA	278	A	C5-C6-N1	5.02	120.21	117.70
26	BA	2662	A	C4-C5-N7	-5.01	108.19	110.70
26	BA	1301	A	C4-C5-N7	-5.01	108.19	110.70
26	BA	2142	A	C5-C6-N1	5.01	120.21	117.70
1	AA	608	A	C4-C5-N7	-5.01	108.19	110.70
1	AA	889	A	C5-C6-N1	5.01	120.21	117.70
1	AA	1363	A	C5-C6-N1	5.01	120.20	117.70
1	AA	1507	A	C5-C6-N1	5.01	120.21	117.70
23	AW	9	A	C5-C6-N1	5.01	120.21	117.70
26	BA	750	A	N9-C4-C5	5.01	107.81	105.80
1	AA	814	A	N9-C4-C5	5.01	107.80	105.80
1	AA	918	A	C5-C6-N1	5.01	120.20	117.70
26	BA	1597	A	C5-C6-N1	5.01	120.20	117.70
26	BA	2560	A	N9-C4-C5	5.01	107.80	105.80
26	BA	756	A	C5-C6-N1	5.01	120.20	117.70
26	BA	2598	A	C8-N9-C4	5.01	107.80	105.80
1	AA	329	A	N9-C4-C5	5.01	107.80	105.80
1	AA	371	A	C5-C6-N1	5.01	120.20	117.70
26	BA	5	A	C5-C6-N1	5.00	120.20	117.70
1	AA	451	A	C5-C6-N1	5.00	120.20	117.70
26	BA	207	A	C5-C6-N1	5.00	120.20	117.70
26	BA	466	A	C8-N9-C4	5.00	107.80	105.80
26	BA	2799	A	N9-C4-C5	5.00	107.80	105.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	BD	151	THR	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	33015	0	16618	253	0
2	AB	1704	0	1732	31	0
3	AC	1624	0	1696	37	0
4	AD	1643	0	1707	74	0
5	AE	1105	0	1148	24	0
6	AF	817	0	808	12	0
7	AG	1181	0	1238	21	0
8	AH	979	0	1031	18	0
9	AI	1022	0	1070	25	0
10	AJ	786	0	828	32	0
11	AK	877	0	887	25	0
12	AL	955	0	1016	20	0
13	AM	883	0	941	22	0
14	AN	774	0	824	26	0
15	AO	710	0	728	7	0
16	AP	649	0	666	22	0
17	AQ	648	0	691	17	0
18	AR	455	0	478	7	0
19	AS	637	0	665	15	0
20	AT	665	0	714	18	0
21	AU	425	0	449	7	0
22	AV	218	0	109	3	0
23	AW	1593	0	820	8	0
24	AX	1656	0	849	10	0
25	AY	1525	0	780	11	0
26	BA	62195	0	31280	430	0
27	BB	2529	0	1281	22	0
28	BC	2082	0	2154	53	0
29	BD	1565	0	1616	40	0
30	BE	1552	0	1619	32	0
31	BF	1410	0	1444	23	0
32	BG	1323	0	1371	27	0
33	BH	359	0	381	13	0
34	BI	1032	0	1085	26	0
35	BJ	1129	0	1162	22	0
36	BK	938	0	1012	26	0
37	BL	1045	0	1117	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BM	1074	0	1157	25	0
39	BN	960	0	1000	29	0
40	BO	892	0	923	21	0
41	BP	917	0	962	22	0
42	BQ	947	0	1019	11	0
43	BR	816	0	839	15	0
44	BS	857	0	922	13	0
45	BT	738	0	807	14	0
46	BU	779	0	831	23	0
47	BV	753	0	780	9	0
48	BW	569	0	581	15	0
49	BX	625	0	652	13	0
50	BY	509	0	543	8	0
51	BZ	449	0	488	10	0
52	B0	444	0	458	8	0
53	B1	409	0	440	12	0
54	B2	377	0	418	7	0
55	B3	504	0	572	15	0
56	B4	302	0	343	8	0
57	B5	74	0	74	23	0
58	AW	9	0	12	3	0
59	BA	51	0	67	12	0
All	All	146760	0	97903	1470	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1470) 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)
59:BA:9000:ERY:C27	57:B5:-2:ASN:ND2	2.18	1.07
59:BA:9000:ERY:H271	57:B5:-2:ASN:HD21	1.13	1.06
59:BA:9000:ERY:H271	57:B5:-2:ASN:ND2	1.74	1.01
59:BA:9000:ERY:C27	57:B5:-2:ASN:HD21	1.72	0.98
58:AW:101:LYS:N	24:AX:76:A:HO2'	1.69	0.91
26:BA:1782:U:C4	57:B5:-4:MET:HE2	2.10	0.86
4:AD:11:LEU:HB3	4:AD:63:ARG:HD3	1.62	0.81
26:BA:1782:U:N3	57:B5:-4:MET:CE	2.43	0.81
4:AD:100:ASN:OD1	4:AD:111:ARG:NH1	2.13	0.79
1:AA:664:G:H22	1:AA:741:G:H1	1.32	0.78
13:AM:66:GLU:HG3	13:AM:67:GLY:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:B2:39:ARG:HG3	54:B2:41:ARG:H	1.50	0.77
40:BO:40:ILE:HG12	40:BO:47:VAL:HG12	1.68	0.76
1:AA:1127:G:H1	1:AA:1145:A:H61	1.35	0.75
30:BE:146:VAL:HG12	30:BE:185:LYS:HB2	1.70	0.74
20:AT:5:LYS:HG3	20:AT:7:ALA:H	1.53	0.74
10:AJ:45:ARG:HB3	10:AJ:69:THR:HB	1.69	0.73
29:BD:151:THR:HG22	29:BD:152:PRO:HD2	1.69	0.73
23:AW:25:C:H42	23:AW:45:G:H22	1.34	0.73
26:BA:1782:U:C4	57:B5:-4:MET:CE	2.72	0.72
10:AJ:49:PHE:HB2	10:AJ:65:TYR:HB2	1.71	0.72
4:AD:95:GLU:HA	4:AD:100:ASN:HD22	1.55	0.72
1:AA:439:U:H4'	4:AD:121:LYS:HD2	1.72	0.72
26:BA:1782:U:C2	57:B5:-4:MET:HE1	2.25	0.71
26:BA:136:G:H1	26:BA:143:C:H42	1.39	0.71
28:BC:107:PRO:HG2	28:BC:110:LEU:HB2	1.73	0.71
30:BE:126:VAL:HG13	30:BE:133:LEU:HD22	1.72	0.71
4:AD:58:LYS:NZ	4:AD:59:GLN:OE1	2.23	0.70
1:AA:1522:U:H5"	11:AK:128:ARG:HH22	1.56	0.70
1:AA:407:U:H2'	1:AA:408:A:H8	1.56	0.70
7:AG:113:ASP:HB2	7:AG:119:ARG:HG2	1.73	0.70
26:BA:1779:U:OP2	26:BA:1784:A:N6	2.24	0.70
3:AC:14:ILE:HG22	3:AC:15:VAL:HG13	1.74	0.70
40:BO:31:THR:O	40:BO:102:ARG:NH1	2.25	0.70
41:BP:33:VAL:HG12	41:BP:35:GLY:H	1.57	0.69
4:AD:95:GLU:OE1	4:AD:100:ASN:ND2	2.25	0.69
35:BJ:118:MET:HA	35:BJ:121:LYS:HE2	1.73	0.69
37:BL:93:ASN:O	37:BL:95:LEU:N	2.24	0.69
1:AA:1359:C:O2'	1:AA:1361:G:N7	2.25	0.69
1:AA:1124:G:O2'	1:AA:1145:A:N6	2.24	0.69
1:AA:438:U:O2'	1:AA:493:A:N6	2.26	0.69
6:AF:91:ARG:HH21	6:AF:93:LYS:HD3	1.58	0.69
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.57	0.69
26:BA:1062:G:H21	34:BI:135:SER:HB3	1.58	0.69
6:AF:90:MET:SD	18:AR:61:ARG:NH1	2.66	0.68
26:BA:1782:U:N3	57:B5:-4:MET:HE1	2.07	0.68
36:BK:21:CYS:HA	36:BK:41:ILE:HG22	1.76	0.68
12:AL:34:CYS:HA	12:AL:55:VAL:HA	1.76	0.68
34:BI:49:ILE:HG13	34:BI:50:GLU:H	1.59	0.68
10:AJ:25:ILE:HD11	10:AJ:87:LEU:HG	1.76	0.68
26:BA:45:G:H5"	26:BA:46:G:H5'	1.77	0.67
26:BA:807:U:OP2	37:BL:41:ARG:NH1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BF:117:LEU:HD13	31:BF:176:PRO:HG2	1.76	0.67
43:BR:6:GLN:HB3	43:BR:37:GLU:HB3	1.76	0.67
48:BW:37:ILE:HG22	48:BW:38:VAL:HG23	1.75	0.67
1:AA:1491:G:H5"	12:AL:43:LYS:HG2	1.76	0.67
26:BA:2728:U:HO2'	26:BA:2729:G:H8	1.41	0.67
1:AA:407:U:H2'	1:AA:408:A:C8	2.30	0.67
36:BK:43:ILE:HD12	36:BK:56:ASP:HB2	1.76	0.67
5:AE:81:LEU:HD13	5:AE:123:VAL:HG11	1.77	0.67
10:AJ:46:LYS:HG2	10:AJ:68:ARG:HG2	1.77	0.67
30:BE:58:LYS:NZ	30:BE:70:SER:O	2.28	0.67
1:AA:570:G:O6	1:AA:865:A:N6	2.28	0.66
14:AN:13:ARG:HE	14:AN:59:ARG:HE	1.43	0.66
51:BZ:10:THR:HG23	51:BZ:11:ARG:HG3	1.77	0.66
20:AT:73:ALA:HA	20:AT:76:LYS:HG2	1.78	0.66
26:BA:1394:U:H4'	26:BA:1603:A:H4'	1.77	0.66
56:B4:19:ARG:HD2	56:B4:24:ARG:HD2	1.77	0.66
2:AB:219:ALA:O	2:AB:222:ARG:NH1	2.29	0.66
31:BF:63:GLN:HE21	31:BF:95:ARG:HH11	1.43	0.66
1:AA:1373:G:H5"	7:AG:36:LYS:HE2	1.78	0.65
3:AC:34:ASP:OD2	14:AN:65:ARG:NH1	2.30	0.65
20:AT:69:LYS:HG3	20:AT:70:ASN:H	1.61	0.65
34:BI:34:ASN:HB3	34:BI:37:GLU:HG2	1.78	0.65
45:BT:59:ASN:HB2	45:BT:84:TYR:HB2	1.78	0.65
55:B3:24:HIS:HD2	55:B3:50:VAL:HG22	1.62	0.65
26:BA:1082:U:H5'	34:BI:119:GLY:HA2	1.78	0.65
1:AA:614:C:OP1	4:AD:83:LYS:NZ	2.30	0.65
29:BD:3:GLY:HA3	29:BD:204:LYS:HG2	1.78	0.65
13:AM:101:ARG:NH1	13:AM:104:THR:OG1	2.29	0.65
49:BX:17:ASN:HB2	49:BX:25:THR:HB	1.77	0.65
1:AA:237:G:H4'	17:AQ:27:ARG:HH12	1.61	0.65
26:BA:482:A:H4'	46:BU:45:HIS:HE1	1.62	0.65
57:B5:-8:ALA:O	57:B5:-6:PHE:N	2.24	0.65
26:BA:2495:G:OP1	38:BM:81:ARG:NH1	2.30	0.65
28:BC:67:PHE:HZ	28:BC:87:ARG:HH22	1.42	0.65
14:AN:3:LYS:HD2	14:AN:6:MET:HG2	1.78	0.64
2:AB:130:THR:HG22	2:AB:132:LYS:H	1.62	0.64
26:BA:2062:A:H8	57:B5:-2:ASN:H	1.44	0.64
1:AA:1221:G:H4'	19:AS:77:THR:HG21	1.78	0.64
3:AC:11:ARG:NH1	3:AC:180:ALA:O	2.30	0.64
1:AA:10:A:OP2	5:AE:131:THR:OG1	2.16	0.64
26:BA:682:G:O6	26:BA:794:A:N6	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BC:210:ALA:O	28:BC:214:ARG:NH1	2.31	0.64
23:AW:75:C:O2'	26:BA:2573:C:N4	2.31	0.64
26:BA:1154:G:OP2	42:BQ:58:ARG:NH1	2.31	0.64
38:BM:11:LYS:HD3	38:BM:86:LYS:HD3	1.80	0.64
59:BA:9000:ERY:H273	57:B5:-2:ASN:ND2	2.12	0.63
36:BK:80:ASP:HB2	41:BP:68:GLU:HB2	1.80	0.63
2:AB:166:ALA:HB3	2:AB:191:SER:HB3	1.81	0.63
29:BD:46:ARG:HB3	29:BD:84:LEU:HD12	1.81	0.63
26:BA:1226:A:OP1	42:BQ:16:LYS:NZ	2.32	0.63
1:AA:243:A:H4'	1:AA:244:U:H3'	1.81	0.63
1:AA:405:U:O4	4:AD:2:ALA:N	2.32	0.63
1:AA:717:U:H4'	11:AK:119:ASN:HD22	1.63	0.63
6:AF:27:ALA:O	6:AF:30:THR:OG1	2.15	0.63
26:BA:335:C:O2	46:BU:68:SER:OG	2.16	0.63
26:BA:863:A:OP1	38:BM:22:GLN:NE2	2.32	0.63
7:AG:71:PRO:O	7:AG:96:ARG:NH1	2.32	0.63
32:BG:164:TYR:HB2	32:BG:167:GLU:HG2	1.79	0.63
1:AA:19:A:OP1	5:AE:135:ASN:ND2	2.32	0.63
1:AA:1072:G:O6	1:AA:1102:A:N6	2.32	0.63
5:AE:77:ASN:HB2	5:AE:82:GLN:HG2	1.81	0.63
1:AA:970:C:OP1	10:AJ:59:LYS:NZ	2.32	0.62
26:BA:1614:A:N6	44:BS:92:ARG:O	2.31	0.62
26:BA:2271:G:H5'	48:BW:20:ARG:HG2	1.81	0.62
40:BO:90:VAL:HG23	40:BO:117:PHE:HB3	1.80	0.62
29:BD:131:ASP:O	29:BD:136:ASN:ND2	2.31	0.62
59:BA:9000:ERY:H212	57:B5:-2:ASN:OD1	1.98	0.62
1:AA:403:C:OP2	4:AD:71:GLN:NE2	2.32	0.62
1:AA:1494:G:HO2'	26:BA:1912:A:HO2'	1.46	0.62
5:AE:133:PRO:HA	5:AE:136:VAL:HG12	1.80	0.62
26:BA:2312:U:H2'	31:BF:37:ASN:HD21	1.63	0.62
28:BC:133:ARG:O	28:BC:167:ARG:NH1	2.32	0.62
26:BA:877:A:O2'	26:BA:900:A:N6	2.32	0.62
36:BK:105:ARG:NH2	41:BP:41:GLN:OE1	2.33	0.62
17:AQ:70:THR:HG22	17:AQ:71:LYS:H	1.63	0.62
26:BA:1788:C:OP1	28:BC:221:ARG:NH2	2.33	0.62
41:BP:27:GLU:HA	41:BP:44:GLU:HA	1.80	0.62
26:BA:2688:G:N1	26:BA:2720:U:OP2	2.32	0.62
34:BI:8:TYR:HB2	34:BI:59:ILE:H	1.63	0.62
37:BL:79:LEU:HD12	37:BL:113:ALA:H	1.64	0.62
1:AA:978:A:OP2	1:AA:1362:A:N6	2.32	0.61
26:BA:2091:C:H3'	26:BA:2092:U:H5"	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BC:73:GLY:O	28:BC:117:GLN:NE2	2.32	0.61
35:BJ:56:VAL:HB	35:BJ:124:VAL:HA	1.82	0.61
1:AA:1397:C:H42	22:AV:22:A:H3'	1.65	0.61
3:AC:28:GLU:O	3:AC:32:ASN:ND2	2.31	0.61
10:AJ:40:ILE:HD12	10:AJ:73:LEU:HD22	1.81	0.61
27:BB:8:C:O2'	40:BO:25:ARG:NH1	2.33	0.61
29:BD:33:ARG:NH1	29:BD:74:GLU:O	2.33	0.61
11:AK:124:PRO:HB2	11:AK:126:LYS:HG2	1.82	0.61
13:AM:25:VAL:HG23	13:AM:29:ARG:HB3	1.82	0.61
9:AI:123:ARG:NH1	9:AI:124:ARG:O	2.33	0.61
2:AB:146:ASN:OD1	2:AB:147:SER:N	2.33	0.61
1:AA:255:G:H4'	17:AQ:19:LYS:HE3	1.83	0.61
28:BC:235:GLY:O	28:BC:239:ASN:ND2	2.32	0.61
25:AY:19:G:H1	26:BA:2112:G:HO2'	1.49	0.61
26:BA:1789:A:OP2	28:BC:221:ARG:NH1	2.33	0.61
31:BF:131:GLY:HA2	31:BF:153:ASP:HA	1.83	0.61
1:AA:69:G:O6	1:AA:98:A:N6	2.33	0.61
26:BA:2581:G:OP2	26:BA:2581:G:N2	2.32	0.61
39:BN:12:ARG:O	39:BN:17:ARG:NH2	2.34	0.61
26:BA:1343:G:O6	26:BA:1403:A:N6	2.34	0.61
26:BA:2199:A:OP1	49:BX:37:ARG:NH1	2.34	0.61
26:BA:2478:A:O2'	26:BA:2536:G:N2	2.34	0.61
6:AF:21:MET:HG2	6:AF:24:ARG:HH21	1.65	0.60
48:BW:23:VAL:HG13	48:BW:38:VAL:HG22	1.83	0.60
26:BA:2298:A:OP1	31:BF:71:ARG:NH2	2.33	0.60
35:BJ:11:VAL:HG11	35:BJ:50:THR:HA	1.83	0.60
26:BA:320:A:O2'	26:BA:322:A:OP2	2.16	0.60
26:BA:958:U:OP2	38:BM:14:LYS:NZ	2.30	0.60
28:BC:159:GLY:H	28:BC:195:VAL:HG13	1.67	0.60
51:BZ:8:THR:HB	51:BZ:56:LYS:HB3	1.84	0.60
1:AA:1396:A:O2'	5:AE:29:ARG:NH2	2.35	0.60
7:AG:57:SER:HB3	7:AG:60:GLU:HG2	1.84	0.60
26:BA:2898:U:O2'	35:BJ:134:ALA:O	2.18	0.60
3:AC:129:MET:SD	3:AC:132:ARG:NH1	2.75	0.60
6:AF:81:ASN:HB3	6:AF:84:VAL:HG12	1.82	0.60
26:BA:1782:U:C2	57:B5:-4:MET:CE	2.84	0.60
3:AC:185:ASN:OD1	3:AC:186:THR:N	2.35	0.60
26:BA:793:A:OP2	26:BA:2071:A:O2'	2.18	0.60
26:BA:1998:A:OP2	29:BD:141:ARG:NH1	2.35	0.60
1:AA:546:A:H61	4:AD:4:TYR:HA	1.66	0.60
26:BA:1693:U:O2'	28:BC:14:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BC:94:VAL:HG11	28:BC:116:ILE:HD11	1.83	0.60
28:BC:252:THR:HG22	28:BC:253:LYS:HG3	1.84	0.60
56:B4:2:LYS:NZ	56:B4:32:LYS:O	2.28	0.60
26:BA:2279:G:N7	48:BW:14:ARG:NH2	2.50	0.59
28:BC:53:HIS:HA	28:BC:217:ARG:HB2	1.84	0.59
31:BF:106:ILE:HD12	31:BF:139:PRO:HG2	1.84	0.59
53:B1:8:LYS:HG2	53:B1:24:THR:HG22	1.82	0.59
46:BU:74:ASN:ND2	46:BU:77:THR:OG1	2.35	0.59
47:BV:51:GLN:HE22	47:BV:86:LEU:HD21	1.67	0.59
53:B1:50:LYS:HG2	53:B1:51:GLU:H	1.67	0.59
16:AP:20:VAL:HG12	16:AP:35:ARG:HA	1.83	0.59
33:BH:9:VAL:HB	33:BH:13:GLY:HA3	1.82	0.59
1:AA:502:A:H61	1:AA:543:U:H3	1.49	0.59
1:AA:1097:C:OP1	2:AB:139:ARG:NH2	2.31	0.59
27:BB:30:C:H1'	27:BB:57:A:H61	1.67	0.59
26:BA:1226:A:H5'	43:BR:86:GLN:HE22	1.68	0.59
26:BA:1334:G:OP1	45:BT:69:ARG:NH2	2.36	0.59
39:BN:103:ARG:HG2	39:BN:105:GLY:H	1.66	0.59
1:AA:848:C:OP1	2:AB:37:LYS:NZ	2.36	0.59
3:AC:56:VAL:HB	3:AC:67:THR:HB	1.83	0.59
10:AJ:47:GLU:OE1	14:AN:76:LYS:NZ	2.34	0.59
21:AU:4:ILE:HD13	21:AU:19:PHE:HE2	1.68	0.59
26:BA:24:G:O2'	44:BS:78:GLU:O	2.19	0.59
26:BA:2485:G:H5"	38:BM:45:GLN:HE21	1.67	0.59
26:BA:2595:G:N2	26:BA:2598:A:OP2	2.36	0.59
1:AA:926:G:N2	22:AV:16:G:OP1	2.36	0.59
1:AA:1351:U:O4	9:AI:120:LYS:NZ	2.36	0.59
3:AC:157:LEU:O	3:AC:164:ARG:NH2	2.33	0.59
5:AE:154:ALA:HA	5:AE:157:ARG:HB3	1.84	0.59
19:AS:3:ARG:NH2	19:AS:68:GLY:O	2.34	0.59
26:BA:2303:G:O2'	31:BF:121:SER:O	2.21	0.59
28:BC:57:GLY:HA2	28:BC:213:TRP:HA	1.85	0.59
51:BZ:5:ILE:HD13	51:BZ:45:ARG:HH22	1.68	0.59
1:AA:766:A:OP2	1:AA:812:G:N2	2.36	0.58
4:AD:147:GLU:HA	4:AD:150:LYS:HE2	1.85	0.58
26:BA:589:U:O3'	30:BE:90:GLN:NE2	2.36	0.58
1:AA:546:A:OP1	4:AD:70:ARG:N	2.35	0.58
26:BA:463:G:N2	26:BA:466:A:OP2	2.31	0.58
41:BP:90:GLY:O	41:BP:113:ARG:NH1	2.36	0.58
1:AA:436:C:O2	4:AD:154:ARG:NH1	2.36	0.58
2:AB:163:VAL:HG21	2:AB:173:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:97:ILE:HA	11:AK:100:LEU:HD13	1.86	0.58
31:BF:57:LEU:HD13	31:BF:89:VAL:HG23	1.84	0.58
3:AC:180:ALA:HB1	3:AC:203:PHE:HE1	1.68	0.58
1:AA:408:A:H61	1:AA:434:U:H3	1.52	0.58
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.83	0.58
40:BO:71:ALA:HB1	40:BO:106:LEU:HB2	1.85	0.58
53:B1:37:LYS:HG2	53:B1:48:ILE:HG13	1.84	0.58
1:AA:618:C:O2'	16:AP:14:ARG:NH2	2.36	0.58
1:AA:890:G:O2'	1:AA:906:A:N6	2.36	0.58
20:AT:84:ASN:HA	20:AT:87:ALA:HB3	1.86	0.58
1:AA:375:U:O2	16:AP:28:ARG:NH2	2.37	0.58
46:BU:33:LYS:HB3	46:BU:64:ALA:HB1	1.85	0.58
3:AC:22:TRP:HB3	3:AC:59:ARG:H	1.69	0.58
37:BL:81:ASP:O	37:BL:83:ALA:N	2.32	0.58
1:AA:875:U:O2'	8:AH:15:ARG:NH1	2.34	0.58
7:AG:27:VAL:HG12	7:AG:43:VAL:HG21	1.85	0.58
9:AI:92:GLU:OE1	9:AI:95:ARG:NH1	2.37	0.58
26:BA:1601:G:OP1	45:BT:64:LYS:NZ	2.36	0.58
1:AA:544:G:OP2	4:AD:63:ARG:NH2	2.36	0.58
3:AC:59:ARG:HE	3:AC:64:ILE:HD12	1.67	0.58
26:BA:1007:C:OP1	35:BJ:37:ARG:NH2	2.37	0.58
26:BA:1992:G:N2	26:BA:1996:C:O2'	2.37	0.58
49:BX:34:HIS:HD2	49:BX:53:ALA:HB2	1.69	0.58
2:AB:72:THR:HG23	2:AB:95:ARG:HA	1.86	0.57
9:AI:112:GLU:OE2	9:AI:115:LYS:NZ	2.37	0.57
25:AY:18:G:H1	25:AY:55:PSU:H1'	1.69	0.57
1:AA:976:G:N2	1:AA:1362:A:O2'	2.37	0.57
21:AU:14:VAL:HG12	21:AU:16:LEU:H	1.67	0.57
26:BA:2266:A:N6	26:BA:2273:A:OP2	2.36	0.57
45:BT:47:VAL:HG21	45:BT:85:VAL:HG11	1.85	0.57
46:BU:29:LEU:HD12	46:BU:33:LYS:HB2	1.86	0.57
50:BY:16:THR:O	50:BY:20:ASN:ND2	2.37	0.57
2:AB:70:VAL:HB	2:AB:163:VAL:HA	1.86	0.57
23:AW:33:U:O2'	23:AW:34:U8U:N	2.37	0.57
30:BE:76:PRO:HA	30:BE:82:GLY:HA2	1.84	0.57
1:AA:67:C:H2'	1:AA:68:G:C8	2.40	0.57
1:AA:426:U:H4'	4:AD:40:GLN:HA	1.85	0.57
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.38	0.57
46:BU:10:GLU:HA	46:BU:24:LYS:HA	1.86	0.57
1:AA:437:U:H5"	4:AD:149:ALA:HB1	1.86	0.57
1:AA:1359:C:H3'	14:AN:75:ARG:HH22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:1568:G:OP2	28:BC:63:ARG:NH1	2.38	0.57
30:BE:117:ARG:NH2	30:BE:183:PHE:O	2.38	0.57
32:BG:3:ARG:HA	32:BG:6:LYS:HE2	1.86	0.57
41:BP:64:ILE:HA	41:BP:69:GLY:HA2	1.85	0.57
8:AH:106:THR:OG1	8:AH:109:GLY:O	2.19	0.57
26:BA:1450:G:N2	26:BA:1452:G:O6	2.37	0.57
33:BH:4:ILE:HD11	33:BH:44:ILE:HG22	1.86	0.57
36:BK:40:LYS:HA	36:BK:59:LYS:HA	1.87	0.57
1:AA:1020:G:H2'	1:AA:1021:A:H8	1.70	0.57
26:BA:1068:G:O6	26:BA:1073:A:N6	2.34	0.57
32:BG:8:PRO:HB2	32:BG:49:THR:HB	1.86	0.57
41:BP:88:ARG:NH2	41:BP:110:ILE:O	2.36	0.57
52:B0:32:LYS:HE2	52:B0:51:GLY:HA3	1.86	0.57
7:AG:135:VAL:HA	7:AG:138:ARG:HG2	1.87	0.57
19:AS:53:ASN:HB3	19:AS:75:ALA:HB1	1.86	0.57
47:BV:77:VAL:HG23	47:BV:89:ILE:HG12	1.87	0.57
1:AA:404:G:O6	4:AD:2:ALA:N	2.38	0.57
1:AA:451:A:H61	1:AA:481:G:H5'	1.70	0.57
4:AD:14:ARG:HG3	4:AD:56:ARG:HH12	1.69	0.57
7:AG:69:VAL:HG21	7:AG:104:ILE:HD11	1.85	0.57
37:BL:54:GLN:HE21	37:BL:60:ARG:HH12	1.53	0.57
37:BL:74:THR:HG22	37:BL:107:PHE:HB2	1.87	0.57
39:BN:44:LEU:HD23	39:BN:113:ILE:HD13	1.87	0.57
28:BC:244:PRO:O	28:BC:251:GLN:NE2	2.37	0.56
8:AH:18:GLN:HE21	8:AH:70:ALA:HB1	1.70	0.56
26:BA:1266:G:OP2	44:BS:15:GLN:NE2	2.38	0.56
28:BC:52:ARG:HH12	28:BC:247:PRO:HG2	1.70	0.56
28:BC:145:GLU:HB2	28:BC:188:CYS:HB3	1.86	0.56
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.37	0.56
10:AJ:5:ARG:HG3	10:AJ:6:ILE:HG13	1.86	0.56
16:AP:12:LYS:HG2	16:AP:13:LYS:HG2	1.87	0.56
23:AW:53:G:OP1	38:BM:55:ARG:NH1	2.37	0.56
26:BA:600:G:OP1	30:BE:24:ASN:ND2	2.37	0.56
26:BA:1782:U:C5	57:B5:-4:MET:HE2	2.40	0.56
29:BD:46:ARG:NH2	29:BD:88:GLU:O	2.35	0.56
29:BD:121:THR:HG21	29:BD:143:PRO:HB3	1.86	0.56
29:BD:151:THR:O	29:BD:153:GLY:N	2.37	0.56
38:BM:50:ARG:HD3	38:BM:65:ILE:HD11	1.87	0.56
38:BM:109:PRO:HD2	38:BM:112:LEU:HD22	1.86	0.56
46:BU:18:ASP:HB3	46:BU:21:LYS:HD2	1.87	0.56
16:AP:15:PRO:HG2	16:AP:41:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2293:G:H5”	40:BO:94:ARG:HH22	1.70	0.56
1:AA:816:A:OP1	1:AA:1526:G:O2’	2.21	0.56
26:BA:411:G:OP2	26:BA:2406:A:O2’	2.22	0.56
26:BA:1782:U:N3	57:B5:-4:MET:HE2	2.16	0.56
1:AA:972:C:H4’	10:AJ:59:LYS:HD3	1.88	0.56
12:AL:57:LEU:HD12	12:AL:61:PHE:HB2	1.86	0.56
20:AT:27:MET:O	20:AT:30:THR:OG1	2.20	0.56
26:BA:750:A:OP1	26:BA:1615:C:N4	2.37	0.56
26:BA:1716:U:H2’	26:BA:1717:A:H8	1.70	0.56
30:BE:46:GLN:HB2	30:BE:87:ALA:H	1.70	0.56
31:BF:99:PHE:HA	31:BF:102:ARG:HE	1.71	0.56
37:BL:63:LYS:HA	55:B3:13:ARG:HG2	1.86	0.56
1:AA:911:U:OP2	12:AL:94:ARG:NH2	2.35	0.56
26:BA:2313:C:O4’	31:BF:37:ASN:ND2	2.35	0.56
40:BO:26:LEU:N	40:BO:91:SER:O	2.37	0.56
1:AA:689:C:OP2	11:AK:53:ARG:NH2	2.29	0.56
1:AA:859:G:OP2	1:AA:869:G:N1	2.30	0.56
26:BA:479:A:H1’	26:BA:481:G:H5’	1.86	0.56
26:BA:815:C:OP2	43:BR:85:LYS:NZ	2.39	0.56
27:BB:14:U:OP2	27:BB:70:C:O2’	2.24	0.56
6:AF:46:GLN:HA	6:AF:56:LYS:HG2	1.87	0.56
12:AL:114:ARG:HG3	12:AL:119:VAL:HB	1.86	0.56
26:BA:135:U:H3	26:BA:144:A:H61	1.53	0.56
26:BA:2294:G:OP1	40:BO:98:GLN:NE2	2.37	0.56
1:AA:1458:G:H5’	20:AT:27:MET:HB3	1.87	0.55
12:AL:38:TYR:HB2	12:AL:52:VAL:HG13	1.88	0.55
26:BA:845:A:H61	26:BA:932:U:H3	1.52	0.55
32:BG:28:GLY:HA3	32:BG:79:VAL:HB	1.86	0.55
3:AC:150:LYS:HG3	3:AC:169:ARG:HB3	1.88	0.55
26:BA:370:G:O2’	26:BA:424:G:OP1	2.24	0.55
1:AA:59:A:H5”	1:AA:387:U:H5”	1.88	0.55
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	1.88	0.55
26:BA:1326:U:H2’	26:BA:1327:A:H8	1.71	0.55
26:BA:1653:G:OP2	39:BN:8:ARG:NH2	2.39	0.55
26:BA:2262:U:OP1	48:BW:41:ARG:NH2	2.39	0.55
32:BG:105:LEU:HB2	32:BG:113:VAL:HB	1.88	0.55
7:AG:78:ARG:HB2	7:AG:85:TYR:HB2	1.87	0.55
26:BA:2336:A:H61	48:BW:43:THR:HG21	1.71	0.55
35:BJ:36:LEU:O	35:BJ:121:LYS:NZ	2.24	0.55
54:B2:3:ARG:HG3	54:B2:5:PHE:H	1.70	0.55
1:AA:1013:G:N2	1:AA:1016:A:OP2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:754:C:OP1	15:AO:72:ARG:NH2	2.40	0.55
3:AC:19:ASN:OD1	3:AC:54:ARG:NH2	2.39	0.55
10:AJ:8:ILE:HD11	10:AJ:87:LEU:HD11	1.89	0.55
26:BA:61:C:OP2	50:BY:47:ARG:NH1	2.38	0.55
26:BA:2355:G:O2'	48:BW:24:LYS:NZ	2.40	0.55
1:AA:1239:A:H61	1:AA:1296:C:H2'	1.70	0.55
1:AA:1359:C:OP2	14:AN:75:ARG:NH1	2.40	0.55
10:AJ:80:THR:HG22	10:AJ:82:LYS:H	1.72	0.55
11:AK:88:GLY:H	11:AK:114:THR:HG22	1.70	0.55
26:BA:2384:U:OP2	48:BW:55:ARG:NH2	2.40	0.55
38:BM:36:VAL:HG23	38:BM:129:THR:H	1.72	0.55
1:AA:340:U:OP2	36:BK:98:ARG:NH2	2.39	0.55
1:AA:1064:G:O2'	1:AA:1190:G:N2	2.40	0.55
26:BA:2751:G:OP2	32:BG:3:ARG:NH1	2.40	0.55
26:BA:2796:U:H3	26:BA:2799:A:H61	1.54	0.55
39:BN:114:GLU:OE1	39:BN:118:ARG:NH2	2.40	0.55
32:BG:89:LEU:HD23	32:BG:94:TYR:HB3	1.87	0.55
42:BQ:28:ARG:HH21	42:BQ:38:ALA:HB1	1.70	0.55
45:BT:40:LYS:NZ	45:BT:58:VAL:O	2.30	0.55
1:AA:132:C:H5"	20:AT:69:LYS:HE3	1.89	0.55
4:AD:2:ALA:HA	4:AD:68:LEU:HD11	1.89	0.55
26:BA:2092:U:O2	26:BA:2225:A:O2'	2.24	0.55
35:BJ:45:THR:HB	35:BJ:48:VAL:HB	1.88	0.55
36:BK:30:ARG:NH2	36:BK:37:ASP:OD2	2.39	0.55
1:AA:406:G:N3	4:AD:116:GLN:NE2	2.53	0.54
1:AA:440:C:H42	1:AA:497:G:H1	1.54	0.54
26:BA:1125:G:H5"	56:B4:37:GLN:HE21	1.72	0.54
3:AC:156:ARG:NH1	3:AC:160:ALA:O	2.40	0.54
9:AI:57:MET:O	9:AI:59:GLU:N	2.40	0.54
26:BA:1936:A:H2	26:BA:1943:U:H3	1.53	0.54
47:BV:25:LYS:HG2	47:BV:43:ASP:HA	1.89	0.54
4:AD:91:LEU:HD13	4:AD:191:LEU:HD11	1.89	0.54
14:AN:51:LEU:O	14:AN:53:ARG:N	2.41	0.54
26:BA:210:C:OP1	54:B2:29:GLN:NE2	2.30	0.54
45:BT:1:MET:HB3	45:BT:2:ILE:HD12	1.90	0.54
1:AA:310:G:H5"	16:AP:31:ARG:HB2	1.90	0.54
2:AB:73:LYS:O	2:AB:77:SER:OG	2.24	0.54
8:AH:50:LYS:HG2	8:AH:52:GLU:HG2	1.87	0.54
11:AK:28:ASN:O	11:AK:57:LYS:NZ	2.35	0.54
28:BC:8:PRO:HB3	28:BC:14:ARG:HG3	1.89	0.54
29:BD:16:THR:OG1	29:BD:18:ASP:OD1	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:982:U:H4'	1:AA:983:A:H5'	1.89	0.54
26:BA:1030:C:OP2	38:BM:127:LYS:NZ	2.38	0.54
26:BA:1169:A:H61	26:BA:1178:C:H41	1.54	0.54
26:BA:1817:G:H5"	28:BC:87:ARG:HE	1.72	0.54
37:BL:124:GLY:HA2	37:BL:144:GLU:HA	1.89	0.54
26:BA:1801:A:N6	26:BA:2201:G:O2'	2.33	0.54
26:BA:2029:G:N1	26:BA:2033:A:OP2	2.36	0.54
26:BA:2334:U:H5'	40:BO:12:THR:HB	1.90	0.54
26:BA:2771:C:O2'	29:BD:173:GLN:NE2	2.30	0.54
43:BR:11:GLN:HE22	43:BR:39:LEU:HD22	1.72	0.54
16:AP:42:ILE:O	16:AP:44:SER:N	2.39	0.54
24:AX:76:A:H2	26:BA:2450:A:N3	2.05	0.54
26:BA:2461:A:N6	26:BA:2488:G:O6	2.41	0.54
30:BE:147:LEU:HB2	30:BE:183:PHE:HD2	1.73	0.54
1:AA:1347:G:N7	9:AI:12:ARG:NH2	2.51	0.54
26:BA:2172:U:H4'	26:BA:2173:A:H5'	1.89	0.54
41:BP:75:GLN:HB2	41:BP:78:SER:HB2	1.89	0.54
50:BY:25:GLN:HE22	50:BY:47:ARG:HG2	1.71	0.54
7:AG:111:ARG:O	7:AG:119:ARG:NH2	2.40	0.54
10:AJ:78:GLU:OE2	10:AJ:80:THR:OG1	2.26	0.54
1:AA:1366:C:O2'	10:AJ:62:ARG:NH1	2.30	0.54
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.90	0.53
12:AL:22:PRO:O	12:AL:24:LEU:N	2.37	0.53
16:AP:4:ILE:HG13	16:AP:21:VAL:HG22	1.90	0.53
26:BA:632:A:H2'	26:BA:633:A:H8	1.73	0.53
26:BA:2645:G:OP2	26:BA:2645:G:N2	2.32	0.53
39:BN:43:GLU:OE1	39:BN:46:ARG:NH1	2.38	0.53
39:BN:78:LYS:HG2	39:BN:83:LEU:HG	1.89	0.53
1:AA:954:G:H21	1:AA:1227:A:H61	1.56	0.53
1:AA:1307:U:OP1	13:AM:100:GLN:NE2	2.40	0.53
14:AN:16:LEU:HD22	14:AN:20:TYR:CE2	2.43	0.53
24:AX:18:G:O2'	24:AX:57:G:N2	2.41	0.53
26:BA:1365:A:OP1	49:BX:28:ARG:NH2	2.40	0.53
59:BA:9000:ERY:C21	57:B5:-2:ASN:OD1	2.56	0.53
26:BA:2489:U:O2'	26:BA:2518:A:N6	2.41	0.53
27:BB:27:C:OP1	40:BO:34:HIS:NE2	2.41	0.53
38:BM:17:ASN:O	38:BM:38:ARG:NH1	2.42	0.53
49:BX:59:ILE:HG12	49:BX:67:VAL:HG21	1.91	0.53
1:AA:115:G:H4'	1:AA:116:A:O5'	2.07	0.53
26:BA:500:G:N1	26:BA:503:A:OP2	2.41	0.53
59:BA:9000:ERY:H271	57:B5:-2:ASN:CG	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B3:39:LYS:HG3	55:B3:42:ARG:HH12	1.74	0.53
1:AA:1494:G:O2'	26:BA:1912:A:O2'	2.23	0.53
4:AD:15:GLU:HG3	4:AD:19:LEU:HD11	1.91	0.53
26:BA:1365:A:O2'	49:BX:11:ARG:NH1	2.41	0.53
26:BA:2343:U:O2'	26:BA:2373:G:O2'	2.25	0.53
20:AT:36:TYR:HA	20:AT:39:ILE:HD12	1.90	0.53
26:BA:2108:A:H4'	26:BA:2150:C:H4'	1.89	0.53
9:AI:95:ARG:HA	9:AI:98:LEU:HB3	1.91	0.53
11:AK:35:THR:HA	11:AK:42:LEU:H	1.73	0.53
13:AM:71:ARG:HH11	31:BF:115:ARG:HH11	1.56	0.53
26:BA:415:A:H61	26:BA:2408:U:H3	1.56	0.53
1:AA:1228:C:OP2	13:AM:110:LYS:NZ	2.31	0.53
26:BA:1326:U:HO2'	26:BA:2010:G:HO2'	1.57	0.53
26:BA:1651:G:N7	39:BN:11:ASN:ND2	2.51	0.53
28:BC:211:ALA:HB1	28:BC:216:VAL:HB	1.91	0.53
36:BK:35:VAL:HG22	36:BK:69:VAL:HG12	1.91	0.53
47:BV:64:VAL:HG22	47:BV:69:GLU:HG2	1.90	0.53
1:AA:1414:U:H2'	1:AA:1415:G:H8	1.74	0.53
26:BA:2250:G:O2'	26:BA:2496:C:OP1	2.26	0.53
26:BA:2377:A:O2'	40:BO:117:PHE:O	2.26	0.53
1:AA:362:G:N2	1:AA:365:U:OP2	2.35	0.53
2:AB:120:GLN:HG3	2:AB:124:GLY:HA3	1.91	0.53
39:BN:96:ARG:HH12	39:BN:116:VAL:HG23	1.74	0.53
40:BO:29:HIS:HB3	40:BO:36:TYR:HB2	1.91	0.53
42:BQ:49:ASP:O	42:BQ:53:ARG:N	2.41	0.53
4:AD:62:ARG:O	4:AD:66:GLY:N	2.40	0.52
8:AH:77:ARG:NH2	8:AH:79:SER:O	2.42	0.52
14:AN:27:LEU:HA	14:AN:31:ILE:HD13	1.91	0.52
17:AQ:31:HIS:HD2	17:AQ:34:TYR:H	1.57	0.52
26:BA:2258:C:O2'	26:BA:2427:C:OP2	2.25	0.52
26:BA:2316:G:H2'	26:BA:2317:A:H8	1.74	0.52
26:BA:2419:U:OP1	55:B3:41:LYS:NZ	2.41	0.52
27:BB:28:C:H2'	27:BB:29:A:C8	2.44	0.52
28:BC:144:VAL:HG11	28:BC:174:LEU:HD21	1.89	0.52
43:BR:10:LYS:HG3	43:BR:12:HIS:CE1	2.45	0.52
1:AA:405:U:O4	4:AD:3:ARG:N	2.43	0.52
43:BR:98:ILE:HG22	43:BR:100:GLY:H	1.74	0.52
26:BA:1613:G:O2'	54:B2:3:ARG:NH1	2.42	0.52
26:BA:1652:A:N6	39:BN:11:ASN:OD1	2.39	0.52
26:BA:2439:A:O4'	57:B5:-3:ARG:NH2	2.39	0.52
28:BC:145:GLU:HA	28:BC:152:GLY:HA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BC:111:LYS:N	28:BC:114:ASP:OD2	2.42	0.52
1:AA:429:U:H5'	4:AD:9:LEU:HB3	1.92	0.52
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.45	0.52
2:AB:128:LYS:HG3	2:AB:129:LEU:HG	1.92	0.52
26:BA:1363:C:H2'	26:BA:1364:G:H8	1.75	0.52
39:BN:69:ARG:O	39:BN:71:ARG:N	2.31	0.52
3:AC:138:VAL:HA	3:AC:149:ILE:HD13	1.90	0.52
26:BA:340:A:O2'	30:BE:162:ARG:NH1	2.42	0.52
44:BS:29:VAL:HG21	44:BS:69:LEU:HG	1.91	0.52
49:BX:33:LEU:HD23	49:BX:50:ARG:HE	1.75	0.52
17:AQ:25:ILE:HB	17:AQ:42:THR:HB	1.92	0.52
26:BA:1028:A:OP2	26:BA:1126:A:N6	2.42	0.52
26:BA:2131:U:H5'	26:BA:2132:U:H5"	1.92	0.52
26:BA:2469:A:O2'	38:BM:55:ARG:NH2	2.36	0.52
28:BC:180:GLU:HB2	28:BC:271:ARG:HB3	1.92	0.52
29:BD:48:ILE:HG23	29:BD:84:LEU:HD21	1.91	0.52
34:BI:12:GLN:HE21	34:BI:55:ILE:H	1.57	0.52
40:BO:20:GLU:OE2	48:BW:62:LYS:NZ	2.41	0.52
40:BO:24:THR:HG22	40:BO:42:PRO:HD3	1.92	0.52
1:AA:111:G:HO2'	1:AA:389:A:HO2'	1.56	0.52
3:AC:19:ASN:ND2	14:AN:90:ARG:O	2.42	0.52
26:BA:1306:C:H41	26:BA:1606:C:H2'	1.75	0.52
26:BA:1515:A:HO2'	26:BA:1556:C:HO2'	1.57	0.52
26:BA:2857:G:N2	26:BA:2860:A:OP2	2.37	0.52
12:AL:54:ARG:HA	12:AL:64:THR:HA	1.91	0.52
17:AQ:17:MET:HG3	17:AQ:20:SER:HB3	1.92	0.52
26:BA:627:A:O4'	26:BA:637:A:N6	2.42	0.52
26:BA:1296:G:OP1	26:BA:2709:G:O2'	2.20	0.52
28:BC:158:ALA:HB1	28:BC:197:ASN:HB3	1.90	0.52
1:AA:689:C:HO2'	1:AA:705:G:HO2'	1.53	0.52
9:AI:107:ASP:OD1	9:AI:109:ARG:NE	2.43	0.51
26:BA:636:G:N2	37:BL:76:GLU:OE2	2.43	0.51
26:BA:1038:G:H2'	26:BA:1039:A:H8	1.74	0.51
26:BA:1796:U:H2'	26:BA:1797:G:H8	1.75	0.51
36:BK:77:ILE:HG12	41:BP:72:ARG:HG2	1.91	0.51
1:AA:350:G:OP1	20:AT:3:ASN:N	2.43	0.51
12:AL:5:ASN:ND2	17:AQ:36:LYS:HE2	2.25	0.51
26:BA:659:G:OP1	30:BE:95:LYS:NZ	2.39	0.51
26:BA:1515:A:H3'	26:BA:1516:G:H8	1.76	0.51
26:BA:1902:C:H5"	28:BC:240:PHE:HE2	1.75	0.51
26:BA:2838:G:H1'	39:BN:45:ARG:HH12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BD:51:THR:HG21	29:BD:68:PHE:HE1	1.75	0.51
31:BF:110:ARG:NH2	31:BF:137:ILE:O	2.43	0.51
1:AA:427:U:OP1	4:AD:13:ARG:NH2	2.43	0.51
3:AC:150:LYS:HB3	3:AC:201:TRP:HB2	1.93	0.51
8:AH:52:GLU:O	8:AH:58:GLU:N	2.42	0.51
20:AT:51:PHE:HA	20:AT:54:MET:HG2	1.92	0.51
23:AW:11:C:H42	23:AW:24:G:H1	1.57	0.51
26:BA:1438:U:H2'	26:BA:1439:A:H8	1.75	0.51
1:AA:563:A:O2'	1:AA:566:G:O3'	2.29	0.51
9:AI:129:LYS:HG3	9:AI:130:ARG:H	1.74	0.51
26:BA:250:G:O5'	37:BL:59:ARG:NH1	2.43	0.51
26:BA:605:G:OP1	30:BE:99:LYS:NZ	2.44	0.51
26:BA:685:A:O2'	26:BA:772:C:N4	2.43	0.51
26:BA:740:C:H5'	26:BA:1784:A:H2'	1.92	0.51
26:BA:1798:U:OP2	28:BC:271:ARG:NH2	2.35	0.51
26:BA:2020:A:H5'	52:B0:9:THR:HG23	1.93	0.51
26:BA:2519:U:O4'	26:BA:2542:A:N6	2.44	0.51
28:BC:123:ALA:O	28:BC:128:ASN:ND2	2.43	0.51
36:BK:2:ILE:HD12	36:BK:8:LEU:HD11	1.93	0.51
41:BP:37:LYS:HE3	41:BP:39:ARG:HB2	1.92	0.51
9:AI:34:SER:OG	9:AI:36:GLU:OE1	2.28	0.51
12:AL:5:ASN:HD21	17:AQ:36:LYS:HE2	1.75	0.51
12:AL:74:LEU:HD21	12:AL:80:ILE:HG21	1.91	0.51
18:AR:57:ARG:HE	18:AR:61:ARG:HH21	1.58	0.51
26:BA:2285:C:H5	53:B1:6:ARG:HH12	1.59	0.51
28:BC:72:ASP:OD2	28:BC:189:ARG:NH1	2.43	0.51
37:BL:57:LEU:HA	37:BL:60:ARG:HG2	1.93	0.51
1:AA:544:G:OP1	4:AD:59:GLN:HG3	2.11	0.51
4:AD:38:PRO:HD2	4:AD:42:GLY:HA3	1.92	0.51
4:AD:50:ASP:O	4:AD:54:GLN:HG2	2.11	0.51
11:AK:94:GLU:OE2	11:AK:98:ARG:NH2	2.44	0.51
26:BA:2080:A:H61	26:BA:2240:U:H3	1.59	0.51
36:BK:15:GLY:HA3	36:BK:50:GLY:HA3	1.93	0.51
1:AA:180:U:O2	1:AA:196:A:N6	2.43	0.51
1:AA:262:A:H5"	20:AT:74:ARG:HH22	1.76	0.51
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.46	0.51
1:AA:380:G:N2	1:AA:383:A:OP2	2.37	0.51
1:AA:954:G:H21	1:AA:1227:A:N6	2.09	0.51
26:BA:805:G:H5"	37:BL:38:GLN:HG3	1.91	0.51
26:BA:1141:U:OP2	35:BJ:65:THR:OG1	2.26	0.51
26:BA:1653:G:O6	39:BN:11:ASN:N	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:2134:A:H8	26:BA:2157:G:H21	1.59	0.51
27:BB:24:G:O2'	27:BB:56:G:N7	2.35	0.51
14:AN:52:PRO:O	14:AN:54:ASP:N	2.37	0.51
26:BA:2441:U:OP2	57:B5:-3:ARG:NH2	2.39	0.51
26:BA:2658:C:OP1	32:BG:158:LYS:NZ	2.43	0.51
32:BG:35:ARG:NH1	32:BG:139:GLN:OE1	2.34	0.51
37:BL:61:LEU:O	55:B3:13:ARG:NE	2.43	0.51
1:AA:1266:G:N2	1:AA:1269:A:OP2	2.39	0.50
9:AI:17:ALA:HB2	9:AI:67:VAL:HG23	1.93	0.50
9:AI:26:GLY:H	9:AI:59:GLU:HG3	1.76	0.50
20:AT:29:ARG:O	20:AT:33:LYS:HG2	2.11	0.50
28:BC:29:PRO:HG2	28:BC:34:LEU:HD11	1.93	0.50
41:BP:48:ILE:HA	41:BP:97:LEU:HD12	1.93	0.50
52:B0:40:ARG:HG2	52:B0:41:HIS:ND1	2.27	0.50
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.46	0.50
12:AL:110:ARG:HH21	12:AL:113:ALA:HB3	1.76	0.50
26:BA:1181:U:H2'	26:BA:1182:G:C8	2.46	0.50
44:BS:41:LYS:HG3	44:BS:43:ALA:H	1.77	0.50
1:AA:458:U:H2'	1:AA:459:A:H8	1.76	0.50
1:AA:1020:G:H2'	1:AA:1021:A:C8	2.46	0.50
30:BE:109:LEU:HD12	30:BE:112:LEU:HD12	1.92	0.50
4:AD:19:LEU:HB3	4:AD:64:ILE:HG12	1.93	0.50
4:AD:104:ARG:HB3	4:AD:168:PRO:HG2	1.92	0.50
5:AE:24:THR:HA	5:AE:29:ARG:HA	1.93	0.50
26:BA:200:U:O4	26:BA:250:G:N2	2.44	0.50
26:BA:373:U:H2'	26:BA:374:A:H8	1.77	0.50
26:BA:1664:A:H61	26:BA:1996:C:H42	1.58	0.50
30:BE:119:ILE:HB	30:BE:187:VAL:HG22	1.93	0.50
1:AA:922:G:H4'	5:AE:25:VAL:HA	1.93	0.50
25:AY:19:G:N1	26:BA:2112:G:O2'	2.44	0.50
26:BA:851:C:O2'	51:BZ:43:ALA:O	2.26	0.50
26:BA:2011:U:OP2	44:BS:16:LYS:NZ	2.41	0.50
29:BD:179:ARG:HB2	29:BD:188:LEU:HD12	1.93	0.50
1:AA:1125:U:H4'	10:AJ:7:ARG:HH12	1.77	0.50
4:AD:167:LYS:HD2	4:AD:173:VAL:HG11	1.92	0.50
26:BA:85:G:OP1	46:BU:7:ARG:N	2.42	0.50
26:BA:2744:G:H21	32:BG:143:GLN:HE22	1.59	0.50
30:BE:111:GLU:OE2	30:BE:114:ARG:NH2	2.45	0.50
46:BU:45:HIS:HB3	46:BU:58:ILE:HA	1.94	0.50
55:B3:28:ASN:HB3	55:B3:36:LYS:HE2	1.94	0.50
1:AA:309:A:H2'	1:AA:310:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:137:U:H3	26:BA:142:A:H61	1.59	0.50
33:BH:40:THR:O	33:BH:42:LYS:N	2.41	0.50
45:BT:7:LEU:HD21	45:BT:46:ALA:HA	1.94	0.50
4:AD:71:GLN:HA	4:AD:74:ASN:HD22	1.76	0.50
13:AM:71:ARG:HA	13:AM:74:SER:HB3	1.93	0.50
26:BA:1564:C:OP2	28:BC:26:LYS:NZ	2.45	0.50
29:BD:181:ASP:HB3	29:BD:186:LEU:HB2	1.94	0.50
50:BY:21:LEU:HA	50:BY:25:GLN:HB2	1.92	0.50
1:AA:765:G:N1	1:AA:812:G:O2'	2.42	0.50
8:AH:103:VAL:HG12	8:AH:126:ILE:HD13	1.93	0.50
10:AJ:27:GLU:HA	10:AJ:30:LYS:HE3	1.93	0.50
26:BA:1034:G:O4'	56:B4:18:LYS:NZ	2.45	0.50
26:BA:1246:A:O2'	30:BE:40:ARG:NH1	2.39	0.50
37:BL:14:LYS:HG3	37:BL:16:GLY:H	1.76	0.50
26:BA:1038:G:H2'	26:BA:1039:A:C8	2.47	0.49
26:BA:1864:U:OP1	26:BA:2410:G:O2'	2.25	0.49
39:BN:28:LEU:HD23	39:BN:48:VAL:HG21	1.93	0.49
4:AD:75:TYR:OH	4:AD:97:ARG:NH1	2.43	0.49
32:BG:24:ILE:HD11	32:BG:43:VAL:HG11	1.94	0.49
32:BG:38:ASN:HB3	32:BG:41:VAL:HG23	1.94	0.49
35:BJ:31:GLU:HG2	35:BJ:142:ILE:HG12	1.93	0.49
35:BJ:40:HIS:CE1	35:BJ:41:LYS:HG3	2.48	0.49
1:AA:809:G:OP2	15:AO:48:LYS:NZ	2.44	0.49
4:AD:29:ASP:O	4:AD:31:LYS:N	2.45	0.49
9:AI:113:ARG:NH1	14:AN:101:TRP:OXT	2.44	0.49
16:AP:71:VAL:O	16:AP:75:ILE:HD12	2.12	0.49
26:BA:1380:G:H21	26:BA:1570:A:H2	1.61	0.49
26:BA:2787:C:H1'	29:BD:63:PRO:HG3	1.94	0.49
34:BI:53:LEU:HD21	34:BI:82:LYS:HE2	1.93	0.49
51:BZ:8:THR:O	51:BZ:56:LYS:N	2.43	0.49
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.76	0.49
17:AQ:24:ALA:HA	17:AQ:43:LYS:HA	1.93	0.49
26:BA:414:C:H2'	26:BA:415:A:C8	2.47	0.49
51:BZ:17:LEU:HB2	51:BZ:20:HIS:HD2	1.77	0.49
9:AI:36:GLU:HA	9:AI:40:GLY:HA3	1.95	0.49
12:AL:3:THR:HG22	12:AL:5:ASN:H	1.77	0.49
59:BA:9000:ERY:C27	57:B5:-2:ASN:CG	2.80	0.49
32:BG:7:ALA:O	32:BG:69:ARG:NE	2.30	0.49
42:BQ:8:VAL:HG13	42:BQ:9:ILE:HG23	1.95	0.49
44:BS:28:LYS:O	44:BS:30:SER:N	2.46	0.49
1:AA:1105:A:H2'	1:AA:1106:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:107:G:H2'	26:BA:108:G:H8	1.78	0.49
26:BA:1662:U:O2'	26:BA:2687:U:OP1	2.31	0.49
26:BA:1817:G:P	28:BC:87:ARG:HH21	2.35	0.49
26:BA:2374:C:N4	26:BA:2375:G:O6	2.45	0.49
26:BA:2845:U:O3'	41:BP:53:ARG:NH1	2.46	0.49
41:BP:25:THR:HB	41:BP:88:ARG:HB3	1.94	0.49
50:BY:31:GLN:HG2	50:BY:37:LEU:HB2	1.94	0.49
26:BA:290:U:H2'	26:BA:291:G:H8	1.77	0.49
26:BA:1996:C:N4	36:BK:32:TYR:OH	2.33	0.49
26:BA:2233:U:H2'	26:BA:2234:G:C8	2.48	0.49
5:AE:25:VAL:HG23	5:AE:27:GLY:H	1.78	0.49
8:AH:9:ASP:O	8:AH:13:ARG:HG2	2.13	0.49
24:AX:76:A:C2	26:BA:2450:A:N3	2.80	0.49
26:BA:2133:G:H2'	26:BA:2157:G:H22	1.78	0.49
28:BC:204:VAL:O	28:BC:206:GLY:N	2.46	0.49
19:AS:28:LYS:HG3	19:AS:29:LYS:H	1.78	0.49
26:BA:1068:G:N2	26:BA:1096:A:OP1	2.45	0.49
26:BA:1131:G:N2	26:BA:1132:U:O4	2.37	0.49
26:BA:1264:A:H5"	52:B0:16:ARG:HH22	1.77	0.49
26:BA:1313:U:H4'	26:BA:1332:G:H4'	1.93	0.49
26:BA:2109:U:O2	26:BA:2181:U:N3	2.45	0.49
51:BZ:17:LEU:HB2	51:BZ:20:HIS:CD2	2.48	0.49
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.95	0.49
1:AA:1313:U:H3	1:AA:1324:A:H61	1.61	0.49
26:BA:246:C:H41	55:B3:8:ARG:HG2	1.78	0.49
26:BA:309:A:H5'	46:BU:17:LYS:HD2	1.94	0.49
26:BA:2134:A:OP2	26:BA:2157:G:N2	2.44	0.49
30:BE:189:THR:HG22	30:BE:191:ASP:H	1.78	0.49
52:B0:31:ASP:HB3	52:B0:35:GLY:H	1.77	0.49
1:AA:321:A:H61	1:AA:332:G:H1	1.61	0.48
1:AA:780:A:N6	1:AA:801:U:OP2	2.42	0.48
58:AW:101:LYS:N	26:BA:2451:A:HO2'	2.11	0.48
25:AY:9:A:N6	25:AY:22:G:N7	2.61	0.48
35:BJ:24:THR:HB	35:BJ:27:ARG:HB2	1.95	0.48
42:BQ:94:ILE:HG21	43:BR:4:VAL:HG21	1.94	0.48
1:AA:28:A:O2'	1:AA:296:U:OP1	2.26	0.48
1:AA:427:U:O2'	1:AA:541:G:OP1	2.32	0.48
1:AA:458:U:H2'	1:AA:459:A:C8	2.49	0.48
26:BA:1666:G:H1	26:BA:1994:C:H42	1.60	0.48
27:BB:116:G:H2'	27:BB:117:G:H8	1.77	0.48
34:BI:62:TYR:HD2	34:BI:67:PHE:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:B1:38:LYS:HB2	53:B1:49:TYR:CE2	2.48	0.48
1:AA:450:G:H4'	16:AP:41:PRO:HB2	1.94	0.48
1:AA:1317:C:N3	14:AN:53:ARG:NH1	2.61	0.48
7:AG:37:SER:HA	7:AG:40:GLU:HG2	1.95	0.48
11:AK:36:ASP:OD1	11:AK:40:ASN:N	2.46	0.48
26:BA:65:U:O3'	45:BT:73:ARG:NH1	2.44	0.48
26:BA:450:G:N1	26:BA:454:A:OP2	2.45	0.48
27:BB:49:C:H2'	27:BB:50:A:H8	1.78	0.48
27:BB:90:C:O3'	38:BM:38:ARG:NH2	2.46	0.48
30:BE:18:THR:HA	30:BE:106:LYS:HD2	1.95	0.48
25:AY:12:U:H3	25:AY:23:A:H61	1.62	0.48
26:BA:1416:G:H1	26:BA:1582:C:H42	1.60	0.48
34:BI:33:VAL:HG13	34:BI:67:PHE:HE2	1.77	0.48
1:AA:512:U:H2'	1:AA:513:C:C6	2.49	0.48
4:AD:9:LEU:HD12	4:AD:12:SER:HB2	1.96	0.48
26:BA:1826:G:O2'	26:BA:1971:U:OP2	2.22	0.48
26:BA:2079:U:O2'	49:BX:23:ASN:OD1	2.26	0.48
26:BA:2316:G:H2'	26:BA:2317:A:C8	2.49	0.48
49:BX:17:ASN:ND2	49:BX:27:ARG:HD2	2.28	0.48
1:AA:1121:U:H3	1:AA:1152:A:H61	1.62	0.48
7:AG:116:MET:HA	7:AG:119:ARG:HD3	1.94	0.48
26:BA:1078:U:O2'	26:BA:1088:A:OP1	2.25	0.48
26:BA:1105:U:H2'	26:BA:1106:G:C8	2.47	0.48
26:BA:1939:U:OP1	26:BA:2604:U:O2'	2.30	0.48
26:BA:2304:G:H4'	31:BF:130:MET:HA	1.96	0.48
26:BA:2359:C:O2'	55:B3:54:ASP:OD2	2.30	0.48
26:BA:2387:U:O2'	48:BW:19:LYS:NZ	2.45	0.48
26:BA:2514:U:H5"	35:BJ:81:ILE:HD11	1.96	0.48
27:BB:22:U:H2'	27:BB:23:G:C8	2.48	0.48
27:BB:43:C:O2	31:BF:92:ARG:NH2	2.38	0.48
31:BF:12:VAL:HG22	31:BF:172:ALA:HB1	1.96	0.48
32:BG:89:LEU:N	32:BG:129:THR:O	2.43	0.48
9:AI:84:THR:HG21	9:AI:103:PHE:HB3	1.95	0.48
15:AO:22:THR:HA	15:AO:27:VAL:HG11	1.94	0.48
20:AT:35:VAL:HG21	20:AT:54:MET:SD	2.54	0.48
26:BA:1077:A:N6	26:BA:1089:A:OP1	2.40	0.48
26:BA:1089:A:H2	26:BA:1090:A:H62	1.62	0.48
26:BA:1187:G:N2	26:BA:1188:U:O4	2.46	0.48
26:BA:1918:A:O2'	26:BA:1920:C:N4	2.47	0.48
1:AA:219:U:H2'	1:AA:220:G:H8	1.79	0.48
1:AA:959:A:HO2'	1:AA:984:C:HO2'	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:95:GLU:HG2	4:AD:186:PRO:HG3	1.94	0.48
11:AK:35:THR:OG1	11:AK:41:ALA:N	2.46	0.48
26:BA:832:U:H2'	26:BA:833:A:C8	2.49	0.48
26:BA:1791:A:N6	26:BA:1828:G:O2'	2.44	0.48
34:BI:34:ASN:OD1	34:BI:35:ILE:N	2.47	0.48
34:BI:79:LEU:HD21	34:BI:109:ILE:HD13	1.94	0.48
34:BI:109:ILE:O	34:BI:112:THR:OG1	2.28	0.48
1:AA:299:G:N2	1:AA:565:U:O2	2.47	0.48
25:AY:32:C:N4	25:AY:33:U:O4	2.47	0.48
26:BA:177:G:OP2	26:BA:177:G:N2	2.29	0.48
26:BA:1570:A:H5'	28:BC:36:LYS:HB2	1.95	0.48
26:BA:2506:U:O2'	26:BA:2507:C:OP1	2.28	0.48
59:BA:9000:ERY:H312	59:BA:9000:ERY:H2	1.66	0.48
27:BB:13:G:O2'	27:BB:15:A:OP2	2.26	0.48
31:BF:128:TYR:OH	31:BF:130:MET:SD	2.67	0.48
33:BH:3:VAL:HG12	33:BH:38:PRO:HA	1.96	0.48
37:BL:79:LEU:HD12	37:BL:114:GLY:H	1.79	0.48
1:AA:429:U:O2'	4:AD:22:LYS:HE2	2.14	0.48
26:BA:673:C:OP1	30:BE:49:ARG:NH2	2.47	0.48
26:BA:1063:G:N2	26:BA:1076:C:O2	2.47	0.48
52:B0:31:ASP:OD2	52:B0:34:SER:N	2.45	0.48
1:AA:202:G:H1	1:AA:215:C:H42	1.61	0.47
1:AA:236:A:H5"	17:AQ:44:LEU:HD21	1.96	0.47
1:AA:512:U:H1'	4:AD:41:HIS:HE1	1.79	0.47
1:AA:1201:A:H4'	1:AA:1202:U:O5'	2.14	0.47
13:AM:16:VAL:HG23	13:AM:17:ILE:HG13	1.96	0.47
13:AM:101:ARG:NH2	13:AM:103:LYS:HD2	2.29	0.47
14:AN:21:PHE:O	14:AN:23:LYS:N	2.47	0.47
37:BL:33:ARG:NH2	37:BL:40:SER:O	2.39	0.47
4:AD:170:TRP:CD1	4:AD:171:LEU:HG	2.49	0.47
9:AI:118:LEU:HG	9:AI:124:ARG:HA	1.96	0.47
32:BG:38:ASN:OD1	32:BG:39:ASP:N	2.47	0.47
32:BG:101:ASN:ND2	32:BG:116:GLN:HE22	2.12	0.47
1:AA:186:C:H5'	20:AT:73:ALA:HB1	1.96	0.47
1:AA:954:G:H1	1:AA:1226:C:H42	1.62	0.47
1:AA:1484:C:HO2'	26:BA:1960:A:HO2'	1.61	0.47
2:AB:66:LYS:NZ	2:AB:154:MET:O	2.39	0.47
5:AE:36:LEU:HD11	5:AE:137:VAL:HG11	1.96	0.47
28:BC:93:LEU:HD11	28:BC:101:ARG:HB3	1.95	0.47
32:BG:35:ARG:HH21	32:BG:71:LEU:HD13	1.79	0.47
39:BN:2:ARG:HA	39:BN:5:LYS:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BZ:7:ILE:N	51:BZ:36:VAL:O	2.46	0.47
1:AA:34:C:N4	1:AA:35:G:O6	2.47	0.47
1:AA:970:C:N4	9:AI:128:SER:OG	2.47	0.47
4:AD:102:VAL:HG13	4:AD:107:PHE:HB2	1.95	0.47
5:AE:88:VAL:HG12	5:AE:93:ARG:HG2	1.96	0.47
26:BA:917:A:H5"	26:BA:2268:A:H61	1.79	0.47
26:BA:2526:G:N3	56:B4:1:MET:N	2.58	0.47
26:BA:2756:U:OP2	56:B4:19:ARG:NE	2.39	0.47
29:BD:151:THR:HG22	29:BD:152:PRO:CD	2.40	0.47
1:AA:178:C:OP2	20:AT:60:ARG:NH2	2.48	0.47
1:AA:1397:C:P	5:AE:29:ARG:HH22	2.37	0.47
3:AC:11:ARG:NH2	3:AC:177:THR:O	2.47	0.47
3:AC:29:PHE:HZ	14:AN:93:ILE:HG23	1.79	0.47
3:AC:189:ALA:HB3	3:AC:196:ILE:HB	1.97	0.47
26:BA:1294:U:O2'	39:BN:23:ASN:OD1	2.27	0.47
29:BD:14:ILE:HG12	29:BD:24:VAL:HG21	1.97	0.47
32:BG:12:PRO:HG2	32:BG:15:VAL:HG21	1.96	0.47
39:BN:50:PRO:O	39:BN:53:THR:OG1	2.25	0.47
1:AA:1265:C:N4	1:AA:1266:G:O6	2.47	0.47
9:AI:99:ARG:NH1	9:AI:105:THR:OG1	2.46	0.47
11:AK:22:HIS:NE2	11:AK:85:MET:SD	2.88	0.47
15:AO:26:GLU:OE2	15:AO:77:ARG:NH2	2.47	0.47
26:BA:442:G:O4'	30:BE:41:GLN:NE2	2.48	0.47
26:BA:475:C:H4'	26:BA:510:C:H5'	1.96	0.47
26:BA:1064:C:H5'	34:BI:90:SER:H	1.79	0.47
44:BS:69:LEU:HA	44:BS:109:ASP:HA	1.97	0.47
45:BT:6:ARG:NH2	45:BT:37:ASP:OD2	2.47	0.47
55:B3:62:LEU:HB3	55:B3:65:ALA:HB2	1.96	0.47
10:AJ:19:ASP:HA	10:AJ:22:THR:HG22	1.97	0.47
19:AS:31:LEU:H	19:AS:49:ILE:HA	1.79	0.47
26:BA:18:U:O2'	26:BA:554:U:OP1	2.30	0.47
26:BA:968:C:H2'	26:BA:969:G:C8	2.49	0.47
26:BA:1790:C:H2'	26:BA:1791:A:C5	2.50	0.47
26:BA:1796:U:H2'	26:BA:1797:G:C8	2.50	0.47
26:BA:2097:A:H61	26:BA:2192:U:H3	1.62	0.47
37:BL:79:LEU:H	37:BL:113:ALA:HB3	1.79	0.47
38:BM:109:PRO:HB2	38:BM:112:LEU:HD13	1.96	0.47
41:BP:53:ARG:N	41:BP:57:SER:OG	2.41	0.47
1:AA:1217:C:OP2	14:AN:9:ARG:NH2	2.47	0.47
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.49	0.47
2:AB:166:ALA:HB2	2:AB:187:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:191:THR:OG1	3:AC:194:GLY:O	2.32	0.47
26:BA:1201:U:H2'	26:BA:1202:G:H8	1.80	0.47
26:BA:2623:G:H2'	26:BA:2624:G:H8	1.79	0.47
28:BC:132:MET:HA	28:BC:135:ILE:HD12	1.96	0.47
29:BD:51:THR:HB	29:BD:79:LEU:HD23	1.97	0.47
46:BU:6:ARG:HG2	46:BU:94:ARG:NH2	2.30	0.47
49:BX:34:HIS:CD2	49:BX:53:ALA:HB2	2.48	0.47
1:AA:1279:G:OP1	10:AJ:9:ARG:NH2	2.48	0.47
3:AC:20:SER:HB3	3:AC:22:TRP:CD1	2.49	0.47
7:AG:25:LYS:O	7:AG:29:ILE:HG12	2.15	0.47
8:AH:13:ARG:HB3	8:AH:25:VAL:HG11	1.97	0.47
9:AI:18:ARG:HH21	9:AI:20:PHE:HZ	1.62	0.47
26:BA:657:U:H2'	26:BA:658:U:C6	2.50	0.47
26:BA:1176:U:H2'	26:BA:1177:G:C8	2.50	0.47
26:BA:2063:C:N4	26:BA:2501:C:O2	2.46	0.47
30:BE:25:GLU:OE2	37:BL:7:SER:N	2.47	0.47
38:BM:64:TRP:HB2	38:BM:104:GLU:HB2	1.96	0.47
41:BP:112:GLU:HG2	41:BP:114:LEU:H	1.80	0.47
47:BV:86:LEU:HD13	47:BV:89:ILE:HD11	1.96	0.47
26:BA:1088:A:N6	34:BI:135:SER:OG	2.47	0.47
26:BA:1578:U:H2'	26:BA:1579:A:H8	1.79	0.47
26:BA:1936:A:OP2	26:BA:1962:C:N4	2.40	0.47
29:BD:2:ILE:HD13	29:BD:90:PHE:HE2	1.80	0.47
29:BD:101:PHE:O	29:BD:104:VAL:HG22	2.16	0.47
32:BG:85:LYS:HG2	32:BG:141:ILE:HD12	1.97	0.47
37:BL:82:LEU:HD13	37:BL:120:VAL:HG21	1.97	0.47
45:BT:11:LEU:HB2	50:BY:26:PHE:HE1	1.80	0.47
1:AA:676:A:H4'	11:AK:115:PRO:HB3	1.96	0.46
1:AA:979:C:H1'	1:AA:1317:C:H41	1.80	0.46
1:AA:1503:A:H5'	1:AA:1531:A:H1'	1.97	0.46
1:AA:56:U:H2'	1:AA:57:G:C8	2.51	0.46
1:AA:950:U:H2'	1:AA:951:G:C8	2.49	0.46
10:AJ:27:GLU:HA	10:AJ:30:LYS:HG2	1.97	0.46
26:BA:1105:U:H2'	26:BA:1106:G:H8	1.80	0.46
26:BA:2286:G:H4'	26:BA:2287:A:C4	2.49	0.46
1:AA:51:A:H61	1:AA:314:C:H1'	1.81	0.46
1:AA:376:G:H4'	16:AP:5:ARG:HD2	1.98	0.46
1:AA:406:G:H2'	1:AA:407:U:C6	2.50	0.46
4:AD:188:ARG:NH2	4:AD:197:GLU:OE1	2.48	0.46
10:AJ:10:LEU:HD22	10:AJ:22:THR:HB	1.97	0.46
14:AN:9:ARG:HG2	14:AN:13:ARG:HH12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BK:98:ARG:HA	36:BK:118:LEU:HD13	1.97	0.46
41:BP:90:GLY:HA2	41:BP:113:ARG:H	1.80	0.46
54:B2:24:THR:HG23	54:B2:27:GLY:H	1.79	0.46
1:AA:335:C:H2'	1:AA:336:A:C8	2.50	0.46
4:AD:145:ILE:HD13	4:AD:178:MET:HB3	1.97	0.46
18:AR:55:LEU:O	18:AR:59:ILE:HG12	2.15	0.46
26:BA:482:A:H4'	46:BU:45:HIS:CE1	2.47	0.46
26:BA:2216:G:H2'	26:BA:2217:G:H8	1.80	0.46
1:AA:376:G:H5"	16:AP:5:ARG:HB2	1.98	0.46
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.51	0.46
8:AH:39:VAL:HG21	8:AH:110:VAL:HG12	1.97	0.46
26:BA:1257:C:H4'	30:BE:78:TRP:CD1	2.51	0.46
26:BA:1365:A:P	49:BX:28:ARG:HH22	2.38	0.46
26:BA:2010:G:H5"	44:BS:42:LYS:HB2	1.98	0.46
26:BA:2106:U:H2'	26:BA:2107:G:C8	2.51	0.46
39:BN:2:ARG:HG3	39:BN:5:LYS:HB2	1.97	0.46
53:B1:13:SER:HA	53:B1:49:TYR:CD1	2.50	0.46
1:AA:501:C:H2'	1:AA:502:A:C8	2.51	0.46
1:AA:539:A:H2'	1:AA:540:G:C8	2.50	0.46
1:AA:675:A:H1'	11:AK:118:HIS:CE1	2.50	0.46
4:AD:83:LYS:O	4:AD:89:ASN:ND2	2.38	0.46
5:AE:45:ARG:HB3	5:AE:71:MET:SD	2.56	0.46
22:AV:15:A:N6	25:AY:34:CM0:O4	2.45	0.46
26:BA:184:C:H2'	26:BA:185:G:H8	1.81	0.46
26:BA:578:G:OP1	26:BA:1255:U:O2'	2.27	0.46
26:BA:1818:U:H2'	28:BC:156:ARG:HB2	1.98	0.46
33:BH:41:LYS:O	33:BH:44:ILE:HG12	2.16	0.46
45:BT:19:LYS:O	45:BT:22:THR:OG1	2.28	0.46
45:BT:23:ALA:O	45:BT:28:ASN:N	2.48	0.46
46:BU:45:HIS:O	46:BU:45:HIS:ND1	2.47	0.46
47:BV:21:ARG:NE	47:BV:87:GLN:OE1	2.47	0.46
53:B1:8:LYS:HD2	55:B3:34:THR:HG21	1.98	0.46
20:AT:35:VAL:HG22	20:AT:50:ALA:HB1	1.96	0.46
26:BA:500:G:OP1	46:BU:43:LYS:NZ	2.45	0.46
26:BA:518:G:O5'	44:BS:18:ARG:NH1	2.49	0.46
26:BA:2744:G:N2	32:BG:143:GLN:HE22	2.13	0.46
29:BD:55:LYS:HB2	29:BD:77:ARG:HA	1.97	0.46
29:BD:112:THR:O	29:BD:195:GLY:HA2	2.15	0.46
34:BI:12:GLN:NE2	34:BI:55:ILE:O	2.49	0.46
43:BR:5:PHE:HB3	43:BR:38:VAL:HG12	1.97	0.46
49:BX:40:VAL:HG11	49:BX:68:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:408:A:H4'	4:AD:109:ALA:HB3	1.98	0.46
1:AA:927:G:OP1	1:AA:1505:G:N2	2.40	0.46
4:AD:14:ARG:HG3	4:AD:56:ARG:NH1	2.30	0.46
14:AN:13:ARG:HE	14:AN:59:ARG:NE	2.12	0.46
26:BA:6:A:HO2'	35:BJ:132:HIS:HD1	1.64	0.46
26:BA:247:G:O2'	26:BA:250:G:O6	2.34	0.46
26:BA:674:G:H1	26:BA:806:C:H42	1.64	0.46
26:BA:1363:C:H2'	26:BA:1364:G:C8	2.51	0.46
28:BC:120:VAL:HG13	28:BC:134:ASN:HD21	1.79	0.46
29:BD:133:THR:OG1	29:BD:134:HIS:N	2.45	0.46
36:BK:25:LEU:O	36:BK:30:ARG:NH1	2.49	0.46
43:BR:14:VAL:HG22	43:BR:15:SER:O	2.16	0.46
49:BX:10:LYS:HE3	49:BX:54:LYS:HD3	1.98	0.46
1:AA:830:G:H2'	1:AA:831:A:H8	1.81	0.46
1:AA:1342:C:H2'	1:AA:1343:G:C8	2.51	0.46
10:AJ:11:LYS:HB2	10:AJ:97:ASP:HB3	1.97	0.46
12:AL:38:TYR:OH	12:AL:54:ARG:NH1	2.48	0.46
26:BA:1802:A:OP2	26:BA:1815:A:N6	2.46	0.46
26:BA:2576:G:O2'	26:BA:2579:C:OP2	2.33	0.46
40:BO:94:ARG:HG3	40:BO:96:GLY:H	1.81	0.46
1:AA:1363:A:O2'	1:AA:1365:G:N7	2.36	0.46
13:AM:64:VAL:O	13:AM:69:LEU:HB2	2.16	0.46
26:BA:281:C:H42	26:BA:359:G:H1	1.64	0.46
26:BA:1199:U:H1'	42:BQ:4:VAL:HG22	1.97	0.46
26:BA:2485:G:H5"	38:BM:45:GLN:NE2	2.30	0.46
59:BA:9000:ERY:H352	59:BA:9000:ERY:H4	1.98	0.46
29:BD:4:LEU:HB2	29:BD:101:PHE:CZ	2.51	0.46
37:BL:78:ARG:NH2	37:BL:80:SER:OG	2.49	0.46
1:AA:219:U:H2'	1:AA:220:G:C8	2.52	0.45
5:AE:150:PRO:HA	5:AE:153:VAL:HG22	1.98	0.45
13:AM:4:ILE:HD11	13:AM:10:PRO:HD2	1.98	0.45
25:AY:65:C:H2'	25:AY:66:A:C8	2.51	0.45
26:BA:2742:G:OP2	56:B4:24:ARG:NH1	2.48	0.45
26:BA:2788:C:H2'	26:BA:2789:C:C6	2.51	0.45
31:BF:13:VAL:O	31:BF:17:MET:HG2	2.17	0.45
1:AA:8:A:H62	4:AD:205:SER:HB2	1.80	0.45
1:AA:971:G:O2'	1:AA:1365:G:O2'	2.30	0.45
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.49	0.45
1:AA:1414:U:H2'	1:AA:1415:G:C8	2.51	0.45
5:AE:137:VAL:O	5:AE:138:ARG:HB2	2.16	0.45
7:AG:105:VAL:O	7:AG:109:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:29:SER:HB2	8:AH:59:LEU:HB2	1.97	0.45
15:AO:36:ILE:O	15:AO:40:GLN:HG2	2.16	0.45
26:BA:806:C:O2	26:BA:2444:G:O2'	2.34	0.45
26:BA:1259:G:H2'	26:BA:1260:A:C8	2.51	0.45
26:BA:1913:A:H4'	26:BA:1914:C:O5'	2.15	0.45
26:BA:2291:U:H2'	26:BA:2292:U:C6	2.52	0.45
48:BW:37:ILE:HD11	48:BW:82:ILE:HD11	1.99	0.45
1:AA:1058:G:OP1	3:AC:199:LYS:NZ	2.46	0.45
2:AB:203:ASN:OD1	2:AB:204:ASP:N	2.50	0.45
3:AC:20:SER:HB3	3:AC:22:TRP:NE1	2.31	0.45
13:AM:31:LYS:NZ	13:AM:41:GLU:OE1	2.49	0.45
26:BA:123:G:H4'	26:BA:1376:C:H5'	1.97	0.45
26:BA:475:C:O2	26:BA:479:A:N6	2.49	0.45
30:BE:75:SER:HB3	30:BE:78:TRP:CE3	2.51	0.45
34:BI:54:PRO:HG2	34:BI:78:VAL:HG21	1.99	0.45
36:BK:64:ARG:NE	41:BP:68:GLU:OE2	2.48	0.45
1:AA:8:A:C6	4:AD:206:LYS:HB3	2.51	0.45
1:AA:263:A:OP1	20:AT:74:ARG:NH1	2.49	0.45
1:AA:1317:C:O2'	14:AN:49:GLN:NE2	2.27	0.45
2:AB:205:ASP:OD1	2:AB:206:ALA:N	2.49	0.45
26:BA:1653:G:C6	39:BN:9:GLN:HB3	2.51	0.45
26:BA:2106:U:H2'	26:BA:2107:G:H8	1.81	0.45
1:AA:12:U:O2'	1:AA:914:A:OP2	2.34	0.45
3:AC:79:LYS:O	3:AC:81:GLY:N	2.48	0.45
4:AD:58:LYS:HD3	4:AD:203:LEU:HD23	1.98	0.45
26:BA:1000:A:OP2	26:BA:1154:G:N1	2.37	0.45
26:BA:2530:A:OP2	26:BA:2535:G:N2	2.50	0.45
28:BC:9:THR:O	28:BC:10:SER:OG	2.28	0.45
30:BE:56:GLY:HA2	30:BE:74:LYS:HZ1	1.81	0.45
33:BH:5:LEU:HD13	33:BH:9:VAL:HG21	1.99	0.45
35:BJ:4:PHE:O	42:BQ:64:ARG:NH2	2.38	0.45
47:BV:10:LYS:HG3	47:BV:11:GLU:HG3	1.99	0.45
1:AA:1320:C:N4	19:AS:37:ARG:HG2	2.32	0.45
26:BA:1010:A:H1'	26:BA:1153:C:H1'	1.99	0.45
26:BA:2223:G:OP1	28:BC:171:TYR:OH	2.24	0.45
26:BA:2772:C:H5'	29:BD:173:GLN:HE21	1.82	0.45
28:BC:162:VAL:HG11	28:BC:174:LEU:HD23	1.98	0.45
36:BK:103:VAL:HB	36:BK:107:LEU:HD22	1.98	0.45
39:BN:32:GLU:HG2	39:BN:115:LEU:HD12	1.97	0.45
39:BN:118:ARG:HH22	52:B0:55:ILE:H	1.63	0.45
41:BP:97:LEU:HB3	41:BP:100:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BV:61:LEU:HB2	47:BV:72:VAL:HG23	1.99	0.45
16:AP:52:LEU:HD21	16:AP:57:ILE:HD12	1.99	0.45
26:BA:1326:U:H2'	26:BA:1327:A:C8	2.50	0.45
27:BB:116:G:H2'	27:BB:117:G:C8	2.51	0.45
29:BD:108:ASP:N	29:BD:204:LYS:O	2.31	0.45
1:AA:939:G:OP1	7:AG:95:ARG:NH2	2.50	0.45
6:AF:5:GLU:OE2	18:AR:23:TYR:OH	2.28	0.45
24:AX:4:G:H1	24:AX:69:U:H3	1.65	0.45
26:BA:250:G:O6	26:BA:386:G:N1	2.38	0.45
26:BA:1597:A:H5"	26:BA:1598:A:H5'	1.98	0.45
26:BA:2719:G:H4'	26:BA:2846:G:H4'	1.98	0.45
26:BA:2840:C:H5"	39:BN:53:THR:HG21	1.98	0.45
27:BB:48:U:P	40:BO:30:ARG:HH22	2.40	0.45
27:BB:95:U:H2'	27:BB:96:G:C8	2.52	0.45
28:BC:166:ALA:HB3	28:BC:173:THR:HB	1.98	0.45
29:BD:4:LEU:HB2	29:BD:101:PHE:HZ	1.81	0.45
36:BK:99:ILE:HD12	36:BK:118:LEU:HD12	1.99	0.45
1:AA:944:G:N1	1:AA:1338:G:OP2	2.32	0.45
3:AC:172:ARG:HG2	3:AC:174:PRO:HD3	1.99	0.45
25:AY:68:C:H2'	25:AY:69:A:H8	1.81	0.45
26:BA:459:U:OP2	54:B2:39:ARG:NH1	2.48	0.45
26:BA:505:A:O2'	26:BA:509:C:O2'	2.21	0.45
26:BA:743:A:O2'	26:BA:1659:G:OP1	2.30	0.45
26:BA:1258:U:H2'	26:BA:1259:G:C8	2.51	0.45
26:BA:1313:U:H2'	26:BA:1313:U:O2	2.16	0.45
26:BA:1651:G:H4'	39:BN:39:PRO:HG2	1.98	0.45
26:BA:2691:C:H2'	26:BA:2692:G:C8	2.52	0.45
34:BI:11:LEU:HD12	34:BI:11:LEU:O	2.16	0.45
1:AA:1217:C:P	14:AN:9:ARG:HH21	2.40	0.45
14:AN:99:ALA:HB1	14:AN:101:TRP:HZ3	1.81	0.45
26:BA:813:U:OP1	43:BR:84:ARG:NH1	2.49	0.45
26:BA:1306:C:H2'	26:BA:1307:A:H8	1.82	0.45
1:AA:1031:C:H4'	1:AA:1032:G:C2	2.52	0.44
1:AA:1060:U:H5"	10:AJ:53:ILE:HG12	1.99	0.44
11:AK:61:PHE:HA	11:AK:64:GLN:HG2	1.97	0.44
14:AN:61:ARG:HE	14:AN:70:PRO:HB2	1.83	0.44
17:AQ:46:VAL:HG13	17:AQ:74:THR:HA	1.99	0.44
26:BA:451:U:O2	26:BA:453:A:N6	2.50	0.44
26:BA:1801:A:OP2	28:BC:150:LYS:NZ	2.38	0.44
26:BA:2170:A:H1'	26:BA:2171:A:C8	2.52	0.44
26:BA:2827:C:H2'	26:BA:2828:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BC:147:LYS:HB2	28:BC:150:LYS:HB2	1.97	0.44
1:AA:254:G:O2'	17:AQ:18:GLU:O	2.35	0.44
1:AA:300:A:O2'	1:AA:564:C:N3	2.48	0.44
1:AA:408:A:H5"	4:AD:110:THR:HG23	1.98	0.44
5:AE:151:GLU:HG3	5:AE:152:MET:HG2	1.99	0.44
10:AJ:9:ARG:NH2	10:AJ:99:GLN:OE1	2.50	0.44
11:AK:112:ASP:OD1	11:AK:114:THR:HG23	2.16	0.44
26:BA:581:C:H2'	26:BA:582:A:C8	2.52	0.44
26:BA:2039:U:H2'	26:BA:2040:G:C8	2.52	0.44
31:BF:37:ASN:OD1	31:BF:38:MET:N	2.50	0.44
33:BH:30:LEU:HB3	33:BH:36:ALA:HB3	1.99	0.44
1:AA:227:G:O2'	16:AP:63:GLN:NE2	2.49	0.44
1:AA:1437:A:H2'	1:AA:1438:G:H8	1.82	0.44
3:AC:8:ASN:HD22	14:AN:90:ARG:HA	1.83	0.44
4:AD:118:VAL:HG11	4:AD:133:ALA:HA	1.98	0.44
11:AK:126:LYS:O	11:AK:127:ARG:HB2	2.18	0.44
17:AQ:27:ARG:HH21	17:AQ:40:ARG:HG2	1.82	0.44
17:AQ:31:HIS:CD2	17:AQ:34:TYR:H	2.34	0.44
26:BA:2298:A:H5"	31:BF:72:LYS:NZ	2.32	0.44
1:AA:830:G:H2'	1:AA:831:A:C8	2.52	0.44
4:AD:28:ILE:HG22	4:AD:30:THR:H	1.83	0.44
13:AM:114:LYS:H	13:AM:115:PRO:HD2	1.82	0.44
17:AQ:60:GLU:OE2	17:AQ:77:ARG:NH2	2.50	0.44
26:BA:619:G:H3'	26:BA:620:G:H21	1.82	0.44
26:BA:1070:A:N6	26:BA:1096:A:O2'	2.51	0.44
26:BA:2874:C:OP1	39:BN:4:ARG:NH2	2.51	0.44
29:BD:104:VAL:O	29:BD:106:LYS:N	2.49	0.44
34:BI:19:ASN:HB2	34:BI:39:CYS:HB3	1.99	0.44
38:BM:33:LEU:HD13	38:BM:117:PHE:HB3	1.98	0.44
2:AB:217:VAL:O	2:AB:221:VAL:HG23	2.18	0.44
13:AM:27:LYS:O	13:AM:31:LYS:HG2	2.17	0.44
23:AW:26:A:H2'	23:AW:27:G:C8	2.53	0.44
30:BE:58:LYS:HA	30:BE:59:PRO:HD3	1.85	0.44
34:BI:61:VAL:HA	34:BI:67:PHE:HB3	1.98	0.44
37:BL:29:LYS:O	37:BL:31:GLY:N	2.51	0.44
43:BR:77:PHE:HD1	43:BR:84:ARG:HB3	1.83	0.44
1:AA:402:G:H2'	1:AA:403:C:C6	2.52	0.44
1:AA:1512:U:H2'	1:AA:1513:A:C8	2.51	0.44
4:AD:162:ALA:O	4:AD:167:LYS:HE3	2.17	0.44
26:BA:2:G:O6	26:BA:2900:A:N6	2.51	0.44
26:BA:379:G:O2'	26:BA:2232:C:OP1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:599:A:H2'	26:BA:600:G:C8	2.52	0.44
26:BA:812:C:H5	37:BL:21:ARG:HB3	1.83	0.44
26:BA:979:A:H2'	26:BA:982:C:H42	1.83	0.44
28:BC:165:VAL:HG11	28:BC:175:ARG:HH21	1.83	0.44
34:BI:94:ASN:ND2	34:BI:137:GLY:HA2	2.32	0.44
46:BU:41:LEU:HB3	46:BU:60:GLU:HG2	1.99	0.44
4:AD:101:VAL:HG21	4:AD:137:VAL:HG21	1.99	0.44
7:AG:73:VAL:HG12	7:AG:90:GLU:HG3	1.99	0.44
24:AX:23:A:H2'	24:AX:24:A:C8	2.53	0.44
26:BA:355:U:H2'	26:BA:356:G:H8	1.83	0.44
26:BA:2621:G:OP1	29:BD:124:ARG:NH2	2.46	0.44
26:BA:2709:G:H5'	39:BN:22:ARG:HH22	1.82	0.44
1:AA:745:G:OP1	1:AA:851:G:O2'	2.36	0.44
2:AB:67:ILE:HD12	2:AB:160:ALA:HB3	2.00	0.44
6:AF:3:HIS:CD2	6:AF:94:HIS:HA	2.53	0.44
9:AI:28:ILE:HG23	9:AI:63:LEU:HD11	1.99	0.44
20:AT:28:MET:HA	20:AT:31:PHE:HD2	1.82	0.44
24:AX:63:C:H2'	24:AX:64:G:C8	2.52	0.44
26:BA:161:A:H3'	26:BA:162:U:H5"	1.99	0.44
26:BA:910:A:H2'	26:BA:911:A:C8	2.53	0.44
26:BA:926:G:H2'	26:BA:927:A:C8	2.52	0.44
26:BA:1106:G:H2'	26:BA:1107:G:H8	1.83	0.44
26:BA:1867:G:H1	26:BA:1874:C:H42	1.66	0.44
26:BA:2368:C:H2'	26:BA:2369:A:C8	2.52	0.44
26:BA:2594:C:N4	26:BA:2595:G:O6	2.51	0.44
30:BE:21:ARG:HH21	30:BE:106:LYS:HE3	1.82	0.44
40:BO:43:ASN:OD1	40:BO:44:GLY:N	2.51	0.44
1:AA:373:A:H61	1:AA:391:G:H1'	1.82	0.43
1:AA:392:C:H2'	1:AA:393:A:C8	2.53	0.43
1:AA:875:U:O3'	8:AH:15:ARG:NH1	2.51	0.43
1:AA:1151:A:O2'	1:AA:1152:A:H5"	2.18	0.43
1:AA:1191:A:H5"	3:AC:4:LYS:HE3	2.00	0.43
3:AC:168:TYR:OH	5:AE:55:GLU:OE2	2.29	0.43
8:AH:95:VAL:HG23	8:AH:102:ALA:HB2	2.00	0.43
21:AU:40:LYS:HB3	21:AU:41:PRO:HD3	1.99	0.43
26:BA:1779:U:H5"	26:BA:1780:A:H5"	2.00	0.43
26:BA:2377:A:H2'	26:BA:2378:A:C8	2.53	0.43
38:BM:75:GLU:HB2	38:BM:90:GLU:HG3	1.99	0.43
2:AB:114:LEU:HD13	2:AB:144:LEU:HB2	2.00	0.43
26:BA:467:G:OP2	54:B2:34:ARG:HD3	2.17	0.43
26:BA:692:C:HO2'	26:BA:1354:A:HO2'	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BE:147:LEU:HB3	30:BE:186:VAL:HG22	2.01	0.43
32:BG:71:LEU:O	32:BG:74:SER:OG	2.28	0.43
39:BN:59:SER:OG	39:BN:62:ASN:OD1	2.35	0.43
4:AD:124:MET:HA	4:AD:129:VAL:HA	1.98	0.43
25:AY:19:G:N2	25:AY:56:C:N3	2.67	0.43
26:BA:215:G:H4'	26:BA:216:A:H4'	2.00	0.43
27:BB:95:U:H2'	27:BB:96:G:H8	1.83	0.43
28:BC:25:HIS:CG	28:BC:80:ARG:HD2	2.53	0.43
28:BC:88:SER:O	28:BC:197:ASN:ND2	2.51	0.43
36:BK:109:SER:O	36:BK:111:LYS:N	2.51	0.43
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.53	0.43
6:AF:10:VAL:HB	6:AF:58:HIS:HB3	2.01	0.43
8:AH:75:ILE:HD12	8:AH:128:TYR:O	2.18	0.43
10:AJ:19:ASP:OD1	10:AJ:20:GLN:N	2.49	0.43
11:AK:23:ILE:HD11	11:AK:86:VAL:HG22	2.00	0.43
11:AK:93:ARG:HH21	21:AU:20:LYS:HG3	1.84	0.43
19:AS:40:ILE:HD13	19:AS:66:MET:HB3	2.00	0.43
26:BA:973:A:H5'	26:BA:1188:U:H1'	2.00	0.43
26:BA:1076:C:H2'	26:BA:1077:A:O4'	2.18	0.43
26:BA:1744:A:H3'	26:BA:1745:A:H8	1.84	0.43
26:BA:1807:G:O2'	26:BA:1809:A:N6	2.51	0.43
26:BA:2279:G:O6	48:BW:14:ARG:NE	2.50	0.43
32:BG:97:ALA:H	32:BG:104:ASN:HB3	1.83	0.43
35:BJ:23:LYS:NZ	35:BJ:142:ILE:OXT	2.51	0.43
53:B1:39:PHE:HA	53:B1:46:HIS:HA	2.00	0.43
1:AA:64:G:H4'	1:AA:65:A:H5"	2.00	0.43
1:AA:960:U:H2'	1:AA:1225:A:H62	1.83	0.43
11:AK:13:ARG:O	11:AK:15:GLN:N	2.46	0.43
12:AL:114:ARG:HH22	12:AL:121:ARG:HH11	1.66	0.43
58:AW:101:LYS:HB3	26:BA:2506:U:O2	2.19	0.43
26:BA:1250:G:OP2	37:BL:21:ARG:NH2	2.52	0.43
26:BA:2548:U:O2	36:BK:23:LYS:NZ	2.50	0.43
34:BI:21:SER:HB3	34:BI:22:PRO:HD3	1.99	0.43
50:BY:21:LEU:HD23	50:BY:25:GLN:HG3	1.99	0.43
55:B3:29:LEU:HA	55:B3:33:LEU:HD21	1.99	0.43
1:AA:403:C:H5'	4:AD:132:ILE:HG23	2.00	0.43
8:AH:92:LEU:HD21	8:AH:113:ASP:HB2	2.01	0.43
32:BG:54:PRO:HG3	32:BG:62:TRP:CD2	2.54	0.43
33:BH:8:LYS:HD3	33:BH:15:LEU:HG	2.00	0.43
52:B0:54:VAL:O	52:B0:56:ALA:N	2.49	0.43
1:AA:1329:A:H5"	13:AM:26:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:152:GLU:HG2	3:AC:167:TRP:HB3	2.00	0.43
11:AK:127:ARG:HB2	21:AU:34:ARG:HE	1.83	0.43
13:AM:11:ASP:OD1	13:AM:12:HIS:N	2.51	0.43
18:AR:29:LEU:HD23	18:AR:59:ILE:HD13	2.00	0.43
26:BA:213:A:H2'	26:BA:214:G:C8	2.54	0.43
26:BA:548:G:O2'	26:BA:549:G:N7	2.51	0.43
26:BA:2093:G:H2'	26:BA:2094:A:H8	1.84	0.43
26:BA:2146:C:O2'	26:BA:2147:A:O5'	2.23	0.43
35:BJ:32:LEU:HD22	35:BJ:54:ILE:HG21	2.00	0.43
51:BZ:6:LYS:HA	51:BZ:37:GLU:HA	1.99	0.43
55:B3:33:LEU:HB3	55:B3:41:LYS:HD3	2.01	0.43
1:AA:252:U:O4	1:AA:253:A:N6	2.46	0.43
2:AB:199:VAL:HG22	2:AB:201:PRO:HD3	2.01	0.43
3:AC:84:VAL:HG13	3:AC:101:ILE:HD13	2.01	0.43
6:AF:50:PRO:HG3	6:AF:55:HIS:CE1	2.53	0.43
23:AW:13:C:H4'	23:AW:14:A:OP1	2.18	0.43
26:BA:53:A:H2	26:BA:179:C:H4'	1.83	0.43
26:BA:572:A:H61	26:BA:2029:G:H21	1.67	0.43
26:BA:632:A:H2'	26:BA:633:A:C8	2.53	0.43
26:BA:720:U:H2'	26:BA:721:A:C8	2.54	0.43
27:BB:24:G:N2	27:BB:28:C:O2	2.51	0.43
30:BE:131:THR:HG22	30:BE:160:ALA:HA	2.00	0.43
35:BJ:77:HIS:HD1	35:BJ:79:GLY:H	1.67	0.43
35:BJ:117:ALA:HA	35:BJ:120:ARG:HH21	1.84	0.43
41:BP:29:LYS:HD2	41:BP:83:SER:HB2	2.01	0.43
53:B1:50:LYS:HG2	53:B1:51:GLU:N	2.33	0.43
1:AA:407:U:O2'	4:AD:113:GLU:HB2	2.19	0.43
2:AB:20:THR:OG1	2:AB:37:LYS:O	2.26	0.43
2:AB:106:THR:O	2:AB:109:GLN:NE2	2.52	0.43
5:AE:80:THR:HB	5:AE:122:ASN:HD21	1.83	0.43
19:AS:8:GLY:HA2	19:AS:9:PRO:HD3	1.90	0.43
26:BA:1254:A:H5"	26:BA:1255:U:H5"	2.01	0.43
26:BA:1266:G:O2'	26:BA:2012:G:O6	2.33	0.43
26:BA:1636:U:H2'	26:BA:1637:A:C8	2.54	0.43
30:BE:55:SER:O	30:BE:74:LYS:NZ	2.52	0.43
44:BS:62:ASP:OD1	44:BS:62:ASP:N	2.51	0.43
2:AB:138:THR:HA	2:AB:141:LEU:HD13	2.01	0.43
4:AD:154:ARG:O	4:AD:158:ALA:N	2.47	0.43
8:AH:104:VAL:HA	8:AH:125:ILE:HA	2.01	0.43
12:AL:38:TYR:N	12:AL:52:VAL:O	2.52	0.43
12:AL:83:ARG:HB2	12:AL:98:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AX:16:U:H5'	24:AX:59:G:H1	1.84	0.43
26:BA:296:U:H2'	26:BA:297:G:C8	2.54	0.43
26:BA:1190:G:H2'	26:BA:1191:G:H8	1.84	0.43
26:BA:2680:U:O2'	29:BD:11:MET:SD	2.77	0.43
27:BB:114:C:H2'	27:BB:115:A:C8	2.53	0.43
31:BF:126:GLY:HA2	31:BF:163:ASP:HA	2.01	0.43
34:BI:33:VAL:HG13	34:BI:67:PHE:CE2	2.54	0.43
43:BR:82:HIS:O	43:BR:82:HIS:ND1	2.52	0.43
1:AA:96:U:H2'	1:AA:97:G:C8	2.54	0.42
1:AA:337:G:H2'	1:AA:338:A:C8	2.54	0.42
1:AA:403:C:OP1	4:AD:134:SER:HB3	2.18	0.42
1:AA:413:G:H1'	1:AA:428:G:N2	2.34	0.42
1:AA:497:G:H2'	1:AA:498:A:C8	2.54	0.42
1:AA:1227:A:H5'	13:AM:110:LYS:NZ	2.34	0.42
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.54	0.42
5:AE:105:ILE:HD13	5:AE:121:HIS:HA	2.00	0.42
7:AG:151:PHE:CE2	11:AK:56:ARG:HG2	2.54	0.42
16:AP:57:ILE:O	16:AP:61:VAL:HG23	2.19	0.42
16:AP:72:ALA:O	16:AP:76:LYS:HG2	2.19	0.42
24:AX:58:A:O2'	24:AX:60:U:OP2	2.24	0.42
26:BA:634:C:H2'	26:BA:635:C:C6	2.54	0.42
26:BA:2002:G:H5"	39:BN:9:GLN:HE21	1.84	0.42
26:BA:2818:U:H2'	26:BA:2819:G:C8	2.53	0.42
29:BD:14:ILE:HA	41:BP:12:GLN:HE22	1.83	0.42
32:BG:83:PHE:HB3	32:BG:141:ILE:HD13	1.99	0.42
38:BM:77:PRO:HB2	38:BM:80:VAL:HG21	2.00	0.42
39:BN:28:LEU:HD22	39:BN:44:LEU:HD21	2.00	0.42
1:AA:408:A:H5"	4:AD:110:THR:CG2	2.49	0.42
26:BA:742:A:H2'	26:BA:743:A:C8	2.54	0.42
26:BA:1469:A:H2'	26:BA:1470:A:C8	2.54	0.42
26:BA:1709:U:H2'	26:BA:1710:G:C8	2.53	0.42
26:BA:1909:C:H2'	26:BA:1910:G:C8	2.54	0.42
26:BA:2537:U:H2'	26:BA:2538:C:C6	2.54	0.42
32:BG:85:LYS:HB2	32:BG:133:LEU:HD11	2.00	0.42
33:BH:8:LYS:HA	33:BH:15:LEU:H	1.83	0.42
41:BP:14:LYS:HE3	41:BP:77:HIS:HA	2.01	0.42
45:BT:37:ASP:OD1	45:BT:37:ASP:N	2.52	0.42
50:BY:31:GLN:O	50:BY:34:SER:OG	2.32	0.42
4:AD:8:LYS:HB3	4:AD:21:LEU:HD13	2.00	0.42
16:AP:18:GLN:HA	16:AP:38:PHE:HA	2.01	0.42
19:AS:36:ARG:NH2	19:AS:72:GLY:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AU:37:PHE:O	21:AU:39:GLU:N	2.51	0.42
23:AW:13:C:O2'	23:AW:14:A:O5'	2.35	0.42
26:BA:629:G:H5"	26:BA:650:C:O2'	2.18	0.42
1:AA:21:G:H2'	1:AA:22:G:C8	2.54	0.42
1:AA:542:G:H2'	1:AA:543:U:C6	2.55	0.42
1:AA:674:G:N2	1:AA:717:U:O2	2.52	0.42
10:AJ:81:GLU:HA	10:AJ:84:VAL:HG12	2.02	0.42
26:BA:269:C:H2'	26:BA:270:A:H8	1.84	0.42
26:BA:322:A:P	30:BE:163:ASN:HD21	2.41	0.42
26:BA:2522:U:O2'	26:BA:2647:U:OP1	2.26	0.42
30:BE:112:LEU:HB3	30:BE:118:LEU:HB2	2.00	0.42
35:BJ:8:PRO:HB3	35:BJ:48:VAL:HG13	2.02	0.42
53:B1:9:ILE:HG21	53:B1:25:LYS:HE2	2.01	0.42
1:AA:495:A:N6	4:AD:116:GLN:HE21	2.17	0.42
1:AA:675:A:OP1	18:AR:74:HIS:NE2	2.53	0.42
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.83	0.42
17:AQ:15:ASP:HB2	17:AQ:55:ILE:HB	2.01	0.42
26:BA:729:G:H5"	26:BA:730:A:H5"	2.01	0.42
26:BA:747:U:O2	26:BA:2014:A:O2'	2.29	0.42
26:BA:2837:A:H2'	26:BA:2838:G:C8	2.55	0.42
29:BD:105:LYS:HG2	29:BD:106:LYS:HG3	2.02	0.42
29:BD:176:ASP:HB2	29:BD:190:LYS:HE2	2.01	0.42
1:AA:1522:U:H2'	1:AA:1523:G:H8	1.85	0.42
13:AM:4:ILE:HD12	13:AM:22:ILE:HD11	2.01	0.42
16:AP:35:ARG:HH21	16:AP:38:PHE:HB3	1.84	0.42
26:BA:922:C:H2'	26:BA:923:G:H8	1.84	0.42
26:BA:1595:C:H2'	26:BA:1596:A:C8	2.55	0.42
26:BA:2097:A:OP2	26:BA:2097:A:H8	2.01	0.42
26:BA:2523:G:HO2'	26:BA:2764:A:HO2'	1.64	0.42
38:BM:41:LEU:HG	38:BM:96:ILE:HG13	2.01	0.42
46:BU:4:LYS:HB3	46:BU:83:VAL:HG21	2.01	0.42
1:AA:52:C:H2'	1:AA:53:A:C8	2.55	0.42
1:AA:587:G:N2	1:AA:754:C:OP2	2.43	0.42
26:BA:84:A:OP2	46:BU:6:ARG:NH1	2.53	0.42
26:BA:371:A:H61	26:BA:401:A:H3'	1.85	0.42
26:BA:1097:U:C4	26:BA:1098:A:H1'	2.55	0.42
26:BA:1899:A:H4'	26:BA:1901:A:H5"	2.01	0.42
2:AB:47:VAL:HB	2:AB:48:PRO:HD3	2.01	0.42
4:AD:168:PRO:HB3	4:AD:170:TRP:CH2	2.55	0.42
5:AE:12:GLN:HB3	5:AE:40:GLY:O	2.19	0.42
7:AG:72:THR:HA	7:AG:96:ARG:HH12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:171:U:H2'	26:BA:172:A:C8	2.55	0.42
26:BA:906:U:O2'	38:BM:66:ARG:NH2	2.41	0.42
26:BA:1903:G:H2'	26:BA:1904:G:H8	1.83	0.42
35:BJ:16:TYR:HE1	35:BJ:138:GLN:HE21	1.68	0.42
43:BR:75:VAL:HG12	43:BR:77:PHE:H	1.85	0.42
1:AA:106:C:H2'	1:AA:107:G:C8	2.54	0.42
1:AA:439:U:H2'	1:AA:440:C:C6	2.55	0.42
1:AA:545:C:H5'	4:AD:69:GLU:CB	2.49	0.42
1:AA:950:U:H2'	1:AA:951:G:H8	1.85	0.42
4:AD:121:LYS:HB3	4:AD:129:VAL:CG2	2.50	0.42
13:AM:5:ALA:H	13:AM:57:ARG:NH1	2.18	0.42
26:BA:573:U:O2'	26:BA:575:A:OP1	2.27	0.42
27:BB:49:C:H2'	27:BB:50:A:C8	2.54	0.42
1:AA:73:C:O2'	1:AA:74:A:H8	2.02	0.42
1:AA:1105:A:H2'	1:AA:1106:G:C8	2.54	0.42
13:AM:17:ILE:O	13:AM:20:THR:OG1	2.23	0.42
19:AS:41:PHE:HB2	19:AS:44:MET:HG3	2.01	0.42
26:BA:1028:A:N6	26:BA:1125:G:H2'	2.34	0.42
26:BA:1178:C:H2'	26:BA:1179:G:H8	1.85	0.42
26:BA:1438:U:H2'	26:BA:1439:A:C8	2.54	0.42
36:BK:15:GLY:O	36:BK:47:ILE:HG13	2.19	0.42
42:BQ:108:ALA:HB1	43:BR:48:LYS:NZ	2.35	0.42
1:AA:995:C:N3	1:AA:1046:A:O2'	2.46	0.41
1:AA:1227:A:H5'	13:AM:110:LYS:HZ2	1.85	0.41
10:AJ:12:ALA:HB3	10:AJ:18:ILE:HB	2.02	0.41
11:AK:31:ILE:HG13	11:AK:46:THR:HG22	2.02	0.41
11:AK:86:VAL:HB	11:AK:112:ASP:HA	2.02	0.41
14:AN:7:LYS:O	14:AN:11:VAL:HG23	2.20	0.41
16:AP:43:ALA:HB1	16:AP:49:GLY:HA2	2.02	0.41
16:AP:46:LYS:HG3	16:AP:47:GLU:HG2	2.02	0.41
17:AQ:61:ILE:HD11	17:AQ:73:TRP:HB3	2.01	0.41
19:AS:11:ILE:HG22	19:AS:39:THR:H	1.84	0.41
26:BA:141:G:OP2	26:BA:142:A:N6	2.53	0.41
26:BA:244:A:OP2	55:B3:8:ARG:NH1	2.51	0.41
26:BA:290:U:H2'	26:BA:291:G:C8	2.55	0.41
26:BA:2355:G:H1'	48:BW:39:ARG:HH21	1.84	0.41
26:BA:2836:U:H2'	26:BA:2837:A:C8	2.55	0.41
29:BD:108:ASP:OD1	29:BD:174:SER:N	2.41	0.41
1:AA:408:A:N6	1:AA:434:U:H3	2.15	0.41
1:AA:891:U:H2'	1:AA:892:A:H8	1.84	0.41
7:AG:73:VAL:HG12	7:AG:90:GLU:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:97:ASN:OD1	7:AG:98:ALA:N	2.53	0.41
9:AI:6:TYR:CE1	9:AI:89:GLU:HG2	2.56	0.41
10:AJ:6:ILE:HG22	10:AJ:8:ILE:HG13	2.02	0.41
19:AS:63:THR:HB	19:AS:66:MET:HG2	2.02	0.41
26:BA:546:U:O2	26:BA:546:U:H2'	2.19	0.41
26:BA:594:U:H2'	26:BA:595:C:C6	2.55	0.41
26:BA:958:U:H5'	38:BM:14:LYS:HE2	2.03	0.41
26:BA:1252:G:H1	42:BQ:37:GLN:HE21	1.67	0.41
26:BA:1668:A:H61	26:BA:1676:A:H61	1.67	0.41
26:BA:2623:G:H2'	26:BA:2624:G:C8	2.54	0.41
59:BA:9000:ERY:H151	59:BA:9000:ERY:H202	1.84	0.41
27:BB:80:U:H2'	27:BB:81:G:H8	1.85	0.41
44:BS:44:ALA:HA	44:BS:47:VAL:HG12	2.02	0.41
1:AA:626:G:OP1	16:AP:35:ARG:NH2	2.48	0.41
1:AA:662:U:O2'	1:AA:836:G:OP1	2.23	0.41
1:AA:1055:A:O2'	3:AC:161:GLU:O	2.34	0.41
1:AA:1222:G:OP2	1:AA:1322:C:N4	2.53	0.41
1:AA:1316:G:N2	1:AA:1319:A:OP2	2.53	0.41
2:AB:68:LEU:O	2:AB:162:PHE:HB3	2.19	0.41
3:AC:35:SER:OG	3:AC:59:ARG:NH2	2.45	0.41
9:AI:7:TYR:HD1	9:AI:20:PHE:HE1	1.67	0.41
11:AK:23:ILE:HG22	11:AK:32:VAL:HG22	2.01	0.41
26:BA:307:G:N1	26:BA:310:A:OP2	2.50	0.41
28:BC:45:ASN:OD1	28:BC:46:ASN:N	2.53	0.41
28:BC:135:ILE:HA	28:BC:136:PRO:HD3	1.89	0.41
34:BI:5:VAL:HA	34:BI:8:TYR:HE2	1.86	0.41
34:BI:80:LEU:HD22	34:BI:136:MET:HE1	2.03	0.41
34:BI:90:SER:HB3	34:BI:93:PRO:HG3	2.03	0.41
1:AA:495:A:N6	4:AD:120:HIS:HE1	2.18	0.41
1:AA:837:U:H2'	1:AA:838:G:H8	1.85	0.41
4:AD:88:GLU:HG2	4:AD:188:ARG:HD3	2.01	0.41
26:BA:249:C:O2	55:B3:12:LYS:NZ	2.54	0.41
26:BA:1012:U:O4	35:BJ:30:THR:HG21	2.20	0.41
26:BA:2286:G:H1	53:B1:23:THR:HG21	1.85	0.41
33:BH:26:ALA:HA	33:BH:30:LEU:HB2	2.01	0.41
36:BK:10:VAL:HG12	36:BK:12:ASP:H	1.85	0.41
36:BK:47:ILE:HA	36:BK:48:PRO:HD3	1.90	0.41
46:BU:74:ASN:HB2	46:BU:79:LYS:O	2.21	0.41
46:BU:86:ARG:H	46:BU:95:PHE:HE2	1.68	0.41
51:BZ:41:THR:OG1	51:BZ:42:PRO:HD2	2.19	0.41
55:B3:17:THR:OG1	55:B3:21:GLY:O	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:235:C:H2'	1:AA:236:A:C8	2.55	0.41
1:AA:409:U:O5'	4:AD:24:GLY:HA3	2.21	0.41
1:AA:658:C:H1'	15:AO:22:THR:HG21	2.03	0.41
7:AG:69:VAL:HA	7:AG:138:ARG:HD3	2.02	0.41
9:AI:83:ILE:O	9:AI:87:LEU:HG	2.20	0.41
14:AN:80:SER:O	14:AN:84:VAL:HG23	2.20	0.41
24:AX:50:C:H2'	24:AX:51:G:C8	2.55	0.41
26:BA:534:U:H2'	26:BA:535:G:C8	2.55	0.41
26:BA:1190:G:H2'	26:BA:1191:G:C8	2.56	0.41
26:BA:2428:G:N2	37:BL:60:ARG:HH22	2.19	0.41
26:BA:2528:U:O2'	26:BA:2530:A:OP1	2.30	0.41
38:BM:13:HIS:O	38:BM:71:LYS:NZ	2.53	0.41
38:BM:42:THR:HA	38:BM:93:VAL:HG12	2.01	0.41
1:AA:426:U:P	4:AD:33:LYS:HD3	2.61	0.41
1:AA:603:U:H2'	1:AA:604:G:C8	2.56	0.41
6:AF:62:MET:HG2	6:AF:64:VAL:HG23	2.03	0.41
26:BA:64:A:H5"	45:BT:77:ARG:HA	2.03	0.41
26:BA:833:A:H2'	26:BA:834:G:C8	2.55	0.41
26:BA:937:C:H2'	26:BA:938:G:C8	2.56	0.41
26:BA:1316:U:H2'	26:BA:1317:G:C8	2.55	0.41
26:BA:1668:A:N6	26:BA:1676:A:H61	2.19	0.41
26:BA:2061:G:H2'	26:BA:2501:C:O2'	2.21	0.41
26:BA:2092:U:P	33:BH:28:ASN:HD21	2.43	0.41
26:BA:2216:G:H2'	26:BA:2217:G:C8	2.55	0.41
32:BG:88:GLN:HA	32:BG:130:GLU:HA	2.02	0.41
34:BI:93:PRO:HB2	34:BI:94:ASN:H	1.66	0.41
36:BK:113:MET:SD	36:BK:116:ILE:HD11	2.60	0.41
41:BP:63:LYS:O	41:BP:70:VAL:N	2.41	0.41
46:BU:82:ARG:O	46:BU:97:LYS:HG2	2.20	0.41
47:BV:29:ILE:HG22	47:BV:88:HIS:CE1	2.56	0.41
1:AA:309:A:H2'	1:AA:310:G:C8	2.56	0.41
2:AB:69:PHE:HB2	2:AB:91:PHE:HB3	2.03	0.41
2:AB:210:VAL:O	2:AB:214:LEU:HB2	2.20	0.41
5:AE:113:ALA:HA	5:AE:116:GLU:HG2	2.03	0.41
15:AO:24:SER:HB3	15:AO:27:VAL:HG23	2.02	0.41
26:BA:5:A:H2'	26:BA:6:A:C8	2.55	0.41
26:BA:668:A:H2'	26:BA:670:A:H62	1.85	0.41
26:BA:1299:G:H5"	26:BA:1300:G:H5"	2.02	0.41
26:BA:1563:U:H2'	26:BA:1564:C:C6	2.56	0.41
26:BA:2478:A:OP2	56:B4:2:LYS:HD3	2.21	0.41
26:BA:2547:A:H4'	36:BK:29:HIS:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BC:30:PHE:CE2	28:BC:32:PRO:HG2	2.55	0.41
29:BD:136:ASN:OD1	29:BD:137:SER:N	2.53	0.41
33:BH:27:ARG:NH1	33:BH:38:PRO:HB3	2.36	0.41
48:BW:27:GLY:HA2	48:BW:67:VAL:HB	2.02	0.41
1:AA:99:C:H2'	1:AA:100:G:C8	2.55	0.41
1:AA:216:U:H2'	1:AA:217:C:C6	2.56	0.41
2:AB:96:TRP:CZ3	2:AB:98:GLY:HA2	2.56	0.41
3:AC:23:PHE:CZ	10:AJ:11:LYS:HE2	2.56	0.41
3:AC:134:MET:HE2	3:AC:168:TYR:HD2	1.86	0.41
21:AU:45:ARG:O	21:AU:49:LYS:HG2	2.20	0.41
26:BA:1902:C:H5"	28:BC:240:PHE:CE2	2.55	0.41
26:BA:2062:A:C8	57:B5:-3:ARG:HA	2.56	0.41
29:BD:49:GLN:NE2	29:BD:79:LEU:HD13	2.36	0.41
36:BK:9:ASN:OD1	36:BK:18:ARG:NH1	2.53	0.41
37:BL:135:ILE:HG22	37:BL:140:GLY:HA3	2.03	0.41
44:BS:2:GLU:HA	44:BS:108:SER:HB3	2.02	0.41
1:AA:8:A:N6	4:AD:202:GLU:O	2.54	0.41
1:AA:728:A:H2'	1:AA:729:A:C8	2.55	0.41
1:AA:784:A:H2'	1:AA:785:G:C8	2.56	0.41
1:AA:1075:U:H2'	1:AA:1076:U:C6	2.56	0.41
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	2.01	0.41
4:AD:34:ILE:O	4:AD:36:GLN:N	2.47	0.41
4:AD:102:VAL:HB	4:AD:114:ALA:HB1	2.03	0.41
4:AD:109:ALA:HB1	4:AD:161:LEU:HD21	2.03	0.41
12:AL:44:LYS:N	12:AL:45:PRO:HD2	2.35	0.41
19:AS:52:HIS:CE1	19:AS:54:GLY:H	2.39	0.41
25:AY:53:G:H1	25:AY:61:C:H42	1.69	0.41
26:BA:45:G:H2'	26:BA:215:G:C5	2.55	0.41
26:BA:172:A:H2'	26:BA:173:A:C8	2.56	0.41
26:BA:355:U:H2'	26:BA:356:G:C8	2.55	0.41
26:BA:948:C:H2'	26:BA:949:G:C8	2.56	0.41
26:BA:968:C:H2'	26:BA:969:G:H8	1.86	0.41
26:BA:1378:A:O2'	26:BA:1380:G:OP2	2.25	0.41
26:BA:1528:A:N6	26:BA:1543:G:O2'	2.53	0.41
26:BA:1782:U:C4	57:B5:-4:MET:SD	3.14	0.41
26:BA:2182:U:H2'	26:BA:2183:A:C8	2.56	0.41
26:BA:2255:G:H1	26:BA:2275:C:H42	1.69	0.41
26:BA:2641:G:H2'	26:BA:2642:G:H8	1.85	0.41
28:BC:258:ARG:NH2	28:BC:264:ASP:OD1	2.47	0.41
29:BD:8:LYS:HB2	29:BD:201:LEU:HD11	2.03	0.41
31:BF:130:MET:O	31:BF:154:ILE:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BG:133:LEU:HD21	32:BG:145:ALA:HB2	2.03	0.41
35:BJ:96:ARG:HH21	35:BJ:99:ARG:HG2	1.85	0.41
40:BO:27:VAL:HA	40:BO:93:ASP:HB3	2.02	0.41
40:BO:74:VAL:O	40:BO:78:VAL:HG23	2.21	0.41
1:AA:374:A:H5"	1:AA:452:A:N1	2.36	0.41
1:AA:1073:U:H3	1:AA:1102:A:H61	1.69	0.41
1:AA:1163:A:H2'	1:AA:1164:G:C8	2.56	0.41
1:AA:1538:C:H2'	1:AA:1539:C:C6	2.55	0.41
9:AI:92:GLU:HB3	9:AI:95:ARG:HH12	1.86	0.41
26:BA:480:A:H5"	46:BU:44:LYS:HD2	2.02	0.41
33:BH:27:ARG:HH12	33:BH:38:PRO:HB3	1.85	0.41
1:AA:147:G:H2'	1:AA:148:G:C8	2.56	0.40
1:AA:591:U:H2'	1:AA:592:G:C8	2.56	0.40
2:AB:151:ILE:HA	2:AB:154:MET:HB2	2.02	0.40
3:AC:6:HIS:HA	3:AC:7:PRO:HD3	1.88	0.40
16:AP:6:LEU:HA	16:AP:19:VAL:HA	2.02	0.40
26:BA:721:A:H2'	26:BA:722:A:C8	2.56	0.40
26:BA:1595:C:H2'	26:BA:1596:A:H8	1.86	0.40
1:AA:19:A:H2'	1:AA:20:U:C6	2.57	0.40
1:AA:392:C:H2'	1:AA:393:A:H8	1.86	0.40
1:AA:512:U:H1'	4:AD:41:HIS:CE1	2.56	0.40
1:AA:540:G:H2'	1:AA:541:G:O4'	2.21	0.40
1:AA:1318:A:O2'	19:AS:37:ARG:HD3	2.21	0.40
1:AA:1515:G:H2'	1:AA:1516:G:C8	2.56	0.40
5:AE:149:SER:O	5:AE:153:VAL:HG13	2.22	0.40
6:AF:51:ILE:HG13	6:AF:51:ILE:O	2.22	0.40
10:AJ:78:GLU:HG3	10:AJ:80:THR:H	1.86	0.40
19:AS:50:ALA:HA	19:AS:59:PRO:HA	2.04	0.40
26:BA:948:C:H2'	26:BA:949:G:H8	1.86	0.40
26:BA:2618:G:H21	29:BD:155:VAL:HG21	1.86	0.40
30:BE:18:THR:HG23	30:BE:106:LYS:HG2	2.03	0.40
39:BN:55:ALA:HA	39:BN:80:PHE:CE1	2.56	0.40
1:AA:454:G:H1	1:AA:478:A:H61	1.69	0.40
1:AA:912:C:H5"	12:AL:43:LYS:NZ	2.36	0.40
2:AB:157:LEU:HA	2:AB:158:PRO:HD3	1.90	0.40
5:AE:107:ALA:H	5:AE:112:ARG:NH2	2.19	0.40
26:BA:20:C:H2'	26:BA:21:A:C8	2.57	0.40
26:BA:1437:C:H2'	26:BA:1438:U:C6	2.57	0.40
26:BA:2547:A:H4'	36:BK:29:HIS:CE1	2.56	0.40
27:BB:44:G:H1'	27:BB:47:C:H42	1.85	0.40
31:BF:25:VAL:O	31:BF:28:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BL:96:LYS:HD3	37:BL:103:ILE:HA	2.03	0.40
46:BU:32:GLY:O	46:BU:67:VAL:HG23	2.21	0.40
46:BU:72:ILE:HD13	46:BU:83:VAL:HG22	2.03	0.40
53:B1:12:VAL:HG22	53:B1:51:GLU:HB3	2.03	0.40
1:AA:1268:G:N3	1:AA:1326:U:O2'	2.47	0.40
26:BA:307:G:N2	26:BA:309:A:H3'	2.37	0.40
26:BA:455:C:N3	26:BA:472:A:H2'	2.37	0.40
26:BA:1056:G:H5"	26:BA:1057:A:O4'	2.21	0.40
26:BA:2305:U:C2	31:BF:151:GLY:HA3	2.56	0.40
27:BB:115:A:H2'	27:BB:116:G:C8	2.56	0.40
40:BO:66:GLY:HA2	40:BO:102:ARG:HH22	1.86	0.40
48:BW:33:ALA:N	48:BW:64:ASP:OD1	2.52	0.40
1:AA:709:U:H2'	1:AA:710:G:H8	1.87	0.40
2:AB:193:PRO:HB2	2:AB:194:ASP:H	1.61	0.40
10:AJ:12:ALA:HB2	10:AJ:96:VAL:HG22	2.03	0.40
12:AL:30:LYS:O	12:AL:82:ILE:HG22	2.21	0.40
13:AM:8:ASN:ND2	13:AM:21:SER:HB3	2.37	0.40
26:BA:249:C:OP2	26:BA:2394:C:O2'	2.36	0.40
26:BA:533:G:H5'	42:BQ:24:TYR:CD1	2.56	0.40
26:BA:743:A:OP1	29:BD:135:GLY:HA2	2.22	0.40
26:BA:2799:A:O2'	26:BA:2800:A:H5"	2.22	0.40
38:BM:42:THR:HG22	38:BM:93:VAL:HG12	2.04	0.40
40:BO:92:PHE:HB2	40:BO:117:PHE:CD1	2.57	0.40
43:BR:49:ILE:HB	43:BR:51:VAL:O	2.22	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	216/240 (90%)	190 (88%)	19 (9%)	7 (3%)	4 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	AC	204/233 (88%)	180 (88%)	20 (10%)	4 (2%)	7 41
4	AD	203/206 (98%)	188 (93%)	8 (4%)	7 (3%)	3 31
5	AE	148/167 (89%)	124 (84%)	17 (12%)	7 (5%)	2 22
6	AF	98/135 (73%)	85 (87%)	8 (8%)	5 (5%)	2 20
7	AG	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	22 61
8	AH	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	19 59
9	AI	125/130 (96%)	113 (90%)	6 (5%)	6 (5%)	2 22
10	AJ	96/103 (93%)	82 (85%)	8 (8%)	6 (6%)	1 17
11	AK	115/129 (89%)	99 (86%)	13 (11%)	3 (3%)	5 35
12	AL	121/124 (98%)	108 (89%)	6 (5%)	7 (6%)	1 18
13	AM	112/118 (95%)	104 (93%)	7 (6%)	1 (1%)	17 57
14	AN	92/101 (91%)	79 (86%)	8 (9%)	5 (5%)	2 19
15	AO	86/89 (97%)	79 (92%)	7 (8%)	0	100 100
16	AP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	5 36
17	AQ	78/84 (93%)	64 (82%)	11 (14%)	3 (4%)	3 27
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100 100
19	AS	77/92 (84%)	71 (92%)	5 (6%)	1 (1%)	12 50
20	AT	83/87 (95%)	76 (92%)	4 (5%)	3 (4%)	3 29
21	AU	49/71 (69%)	36 (74%)	8 (16%)	5 (10%)	0 7
28	BC	269/273 (98%)	247 (92%)	16 (6%)	6 (2%)	6 39
29	BD	207/209 (99%)	190 (92%)	15 (7%)	2 (1%)	15 55
30	BE	199/201 (99%)	188 (94%)	9 (4%)	2 (1%)	15 55
31	BF	175/179 (98%)	154 (88%)	16 (9%)	5 (3%)	4 33
32	BG	174/177 (98%)	161 (92%)	10 (6%)	3 (2%)	9 45
33	BH	45/149 (30%)	37 (82%)	4 (9%)	4 (9%)	1 9
34	BI	139/142 (98%)	116 (84%)	15 (11%)	8 (6%)	1 18
35	BJ	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	22 61
36	BK	120/123 (98%)	106 (88%)	9 (8%)	5 (4%)	3 25
37	BL	141/144 (98%)	117 (83%)	16 (11%)	8 (6%)	1 18
38	BM	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	6 39
39	BN	118/127 (93%)	104 (88%)	9 (8%)	5 (4%)	3 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
40	BO	114/117 (97%)	104 (91%)	7 (6%)	3 (3%)	5 35
41	BP	112/115 (97%)	105 (94%)	5 (4%)	2 (2%)	8 43
42	BQ	115/118 (98%)	113 (98%)	2 (2%)	0	100 100
43	BR	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	3 26
44	BS	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	8 42
45	BT	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	6 39
46	BU	100/104 (96%)	82 (82%)	13 (13%)	5 (5%)	2 21
47	BV	92/94 (98%)	87 (95%)	5 (5%)	0	100 100
48	BW	73/85 (86%)	69 (94%)	4 (6%)	0	100 100
49	BX	75/78 (96%)	73 (97%)	2 (3%)	0	100 100
50	BY	61/63 (97%)	56 (92%)	5 (8%)	0	100 100
51	BZ	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	8 43
52	B0	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
53	B1	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	7 40
54	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6 38
55	B3	62/65 (95%)	57 (92%)	5 (8%)	0	100 100
56	B4	36/38 (95%)	32 (89%)	4 (11%)	0	100 100
57	B5	7/9 (78%)	3 (43%)	3 (43%)	1 (14%)	0 4
All	All	5522/5993 (92%)	4968 (90%)	406 (7%)	148 (3%)	8 35

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	105	ILE
9	AI	55	VAL
11	AK	127	ARG
12	AL	23	ALA
17	AQ	17	MET
17	AQ	51	ASN
21	AU	40	LYS
29	BD	152	PRO
33	BH	3	VAL
33	BH	9	VAL
33	BH	10	ALA
34	BI	93	PRO
37	BL	94	THR

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Mol	Chain	Res	Type
57	B5	-7	VAL
2	AB	193	PRO
4	AD	28	ILE
4	AD	30	THR
5	AE	12	GLN
5	AE	158	GLY
9	AI	13	LYS
9	AI	58	VAL
9	AI	91	ASP
9	AI	129	LYS
10	AJ	57	VAL
10	AJ	101	SER
11	AK	89	PRO
12	AL	34	CYS
12	AL	43	LYS
14	AN	22	ALA
14	AN	52	PRO
14	AN	92	GLU
21	AU	9	ASN
21	AU	24	GLU
31	BF	133	ARG
32	BG	175	LYS
34	BI	13	VAL
34	BI	65	ARG
36	BK	108	ARG
37	BL	29	LYS
37	BL	111	ILE
39	BN	70	THR
39	BN	106	ASP
40	BO	57	ALA
45	BT	77	ARG
46	BU	7	ARG
46	BU	17	LYS
46	BU	76	ALA
2	AB	34	ALA
2	AB	68	LEU
2	AB	82	ASP
3	AC	166	GLU
3	AC	206	GLU
4	AD	175	ALA
5	AE	24	THR
5	AE	101	GLU

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Mol	Chain	Res	Type
6	AF	54	LEU
6	AF	86	ARG
6	AF	94	HIS
7	AG	114	LYS
8	AH	88	ARG
9	AI	9	THR
12	AL	24	LEU
12	AL	76	GLU
12	AL	78	SER
13	AM	114	LYS
14	AN	3	LYS
14	AN	21	PHE
16	AP	43	ALA
16	AP	47	GLU
19	AS	5	LEU
20	AT	41	ALA
21	AU	35	ARG
21	AU	38	TYR
28	BC	240	PHE
32	BG	45	HIS
32	BG	46	ALA
34	BI	88	SER
35	BJ	82	GLY
37	BL	30	THR
37	BL	82	LEU
39	BN	3	HIS
41	BP	36	SER
44	BS	12	SER
51	BZ	4	THR
54	B2	45	SER
2	AB	19	GLN
4	AD	165	ARG
4	AD	192	SER
5	AE	122	ASN
6	AF	63	ASN
10	AJ	95	GLY
12	AL	17	ALA
17	AQ	76	VAL
20	AT	42	GLY
20	AT	68	HIS
28	BC	30	PHE
28	BC	152	GLY

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Mol	Chain	Res	Type
28	BC	253	LYS
29	BD	41	ALA
31	BF	9	LYS
34	BI	31	GLN
36	BK	93	GLN
36	BK	110	GLU
37	BL	70	LYS
38	BM	70	ASP
40	BO	100	HIS
41	BP	94	LYS
43	BR	43	ASN
43	BR	53	PHE
46	BU	55	PRO
46	BU	99	ASN
53	B1	51	GLU
2	AB	75	ALA
6	AF	92	THR
10	AJ	36	VAL
28	BC	205	LEU
28	BC	236	GLU
30	BE	80	SER
30	BE	83	VAL
33	BH	41	LYS
34	BI	21	SER
36	BK	119	ALA
37	BL	100	ILE
38	BM	69	PRO
39	BN	2	ARG
39	BN	118	ARG
40	BO	66	GLY
2	AB	86	SER
4	AD	25	VAL
4	AD	167	LYS
31	BF	175	PHE
31	BF	177	PHE
36	BK	35	VAL
37	BL	4	ASN
38	BM	24	THR
43	BR	7	SER
45	BT	88	LYS
10	AJ	42	LEU
43	BR	58	VAL

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Mol	Chain	Res	Type
44	BS	29	VAL
3	AC	66	VAL
3	AC	81	GLY
10	AJ	41	PRO
5	AE	143	GLY
11	AK	92	GLY
31	BF	149	VAL
34	BI	85	GLY
34	BI	89	GLY

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	180/198 (91%)	180 (100%)	0	100	100
3	AC	170/190 (90%)	170 (100%)	0	100	100
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	113/126 (90%)	113 (100%)	0	100	100
6	AF	87/116 (75%)	87 (100%)	0	100	100
7	AG	124/147 (84%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	105 (100%)	0	100	100
10	AJ	86/90 (96%)	86 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	103/104 (99%)	103 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	75/77 (97%)	75 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AS	70/79 (89%)	70 (100%)	0	100	100
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	44/61 (72%)	44 (100%)	0	100	100
28	BC	216/218 (99%)	216 (100%)	0	100	100
29	BD	164/164 (100%)	164 (100%)	0	100	100
30	BE	165/165 (100%)	165 (100%)	0	100	100
31	BF	148/150 (99%)	148 (100%)	0	100	100
32	BG	137/138 (99%)	137 (100%)	0	100	100
33	BH	38/114 (33%)	38 (100%)	0	100	100
34	BI	109/110 (99%)	109 (100%)	0	100	100
35	BJ	116/116 (100%)	116 (100%)	0	100	100
36	BK	103/104 (99%)	103 (100%)	0	100	100
37	BL	102/103 (99%)	102 (100%)	0	100	100
38	BM	109/109 (100%)	109 (100%)	0	100	100
39	BN	100/103 (97%)	100 (100%)	0	100	100
40	BO	86/87 (99%)	86 (100%)	0	100	100
41	BP	99/100 (99%)	99 (100%)	0	100	100
42	BQ	89/90 (99%)	89 (100%)	0	100	100
43	BR	84/84 (100%)	84 (100%)	0	100	100
44	BS	93/93 (100%)	93 (100%)	0	100	100
45	BT	80/84 (95%)	80 (100%)	0	100	100
46	BU	83/85 (98%)	83 (100%)	0	100	100
47	BV	78/78 (100%)	78 (100%)	0	100	100
48	BW	56/63 (89%)	56 (100%)	0	100	100
49	BX	67/68 (98%)	67 (100%)	0	100	100
50	BY	55/55 (100%)	55 (100%)	0	100	100
51	BZ	48/49 (98%)	48 (100%)	0	100	100
52	B0	47/48 (98%)	47 (100%)	0	100	100
53	B1	45/49 (92%)	45 (100%)	0	100	100
54	B2	38/38 (100%)	38 (100%)	0	100	100
55	B3	51/52 (98%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	B4	34/34 (100%)	34 (100%)	0	100	100
57	B5	8/8 (100%)	8 (100%)	0	100	100
All	All	4594/4885 (94%)	4594 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	15	HIS
3	AC	8	ASN
3	AC	102	ASN
4	AD	41	HIS
4	AD	74	ASN
4	AD	120	HIS
6	AF	37	HIS
6	AF	55	HIS
8	AH	4	GLN
8	AH	16	ASN
11	AK	118	HIS
11	AK	119	ASN
12	AL	5	ASN
12	AL	77	HIS
14	AN	49	GLN
16	AP	63	GLN
17	AQ	31	HIS
19	AS	57	HIS
20	AT	78	ASN
28	BC	46	ASN
28	BC	134	ASN
28	BC	260	ASN
29	BD	150	GLN
29	BD	164	GLN
30	BE	41	GLN
30	BE	92	HIS
30	BE	97	ASN
30	BE	163	ASN
31	BF	63	GLN
32	BG	116	GLN
32	BG	143	GLN
33	BH	43	ASN

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Mol	Chain	Res	Type
34	BI	12	GLN
35	BJ	40	HIS
37	BL	35	HIS
37	BL	54	GLN
38	BM	22	GLN
39	BN	9	GLN
39	BN	73	ASN
42	BQ	20	GLN
42	BQ	37	GLN
43	BR	6	GLN
43	BR	11	GLN
43	BR	86	GLN
44	BS	61	ASN
46	BU	74	ASN
47	BV	51	GLN
49	BX	16	ASN
50	BY	25	GLN
51	BZ	20	HIS
53	B1	19	HIS
55	B3	24	HIS
56	B4	37	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	218 (14%)	4 (0%)
22	AV	9/10 (90%)	0	0
23	AW	70/74 (94%)	13 (18%)	1 (1%)
24	AX	74/77 (96%)	6 (8%)	0
25	AY	67/71 (94%)	13 (19%)	1 (1%)
26	BA	2895/2897 (99%)	425 (14%)	10 (0%)
27	BB	117/120 (97%)	13 (11%)	0
All	All	4769/4788 (99%)	688 (14%)	16 (0%)

All (688) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	8	A
1	AA	9	G

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Mol	Chain	Res	Type
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	70	U
1	AA	74	A
1	AA	81	A
1	AA	83	C
1	AA	85	U
1	AA	87	C
1	AA	88	U
1	AA	95	C
1	AA	97	G
1	AA	108	G
1	AA	116	A
1	AA	120	A
1	AA	121	U
1	AA	130	A
1	AA	131	A
1	AA	149	A
1	AA	182	A
1	AA	204	G
1	AA	207	C
1	AA	208	U
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	279	A
1	AA	280	C
1	AA	289	G
1	AA	298	A
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	347	G

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Mol	Chain	Res	Type
1	AA	352	C
1	AA	354	G
1	AA	356	A
1	AA	367	U
1	AA	372	C
1	AA	378	G
1	AA	397	A
1	AA	406	G
1	AA	409	U
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	436	C
1	AA	437	U
1	AA	451	A
1	AA	452	A
1	AA	459	A
1	AA	467	U
1	AA	468	A
1	AA	478	A
1	AA	479	U
1	AA	482	A
1	AA	485	U
1	AA	486	U
1	AA	496	A
1	AA	497	G
1	AA	509	A
1	AA	511	C
1	AA	518	C
1	AA	527	G
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C

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Mol	Chain	Res	Type
1	AA	577	G
1	AA	596	A
1	AA	633	G
1	AA	642	A
1	AA	650	G
1	AA	665	A
1	AA	675	A
1	AA	687	A
1	AA	702	A
1	AA	703	G
1	AA	721	G
1	AA	723	U
1	AA	731	G
1	AA	747	A
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	829	G
1	AA	832	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	846	G
1	AA	873	A
1	AA	885	G
1	AA	914	A
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	969	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	983	A

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Mol	Chain	Res	Type
1	AA	993	G
1	AA	1004	A
1	AA	1008	U
1	AA	1026	G
1	AA	1027	C
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1034	G
1	AA	1036	A
1	AA	1043	G
1	AA	1044	A
1	AA	1050	G
1	AA	1054	C
1	AA	1065	U
1	AA	1073	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1104	G
1	AA	1125	U
1	AA	1133	G
1	AA	1134	G
1	AA	1136	C
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1145	A
1	AA	1146	A
1	AA	1157	A
1	AA	1159	U
1	AA	1160	G
1	AA	1161	C
1	AA	1196	A
1	AA	1197	A
1	AA	1201	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A

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Mol	Chain	Res	Type
1	AA	1236	A
1	AA	1238	A
1	AA	1240	U
1	AA	1241	G
1	AA	1253	G
1	AA	1256	A
1	AA	1257	A
1	AA	1261	A
1	AA	1275	A
1	AA	1280	A
1	AA	1285	A
1	AA	1286	U
1	AA	1287	A
1	AA	1299	A
1	AA	1300	G
1	AA	1305	G
1	AA	1317	C
1	AA	1318	A
1	AA	1322	C
1	AA	1337	G
1	AA	1346	A
1	AA	1347	G
1	AA	1363	A
1	AA	1364	U
1	AA	1377	A
1	AA	1379	G
1	AA	1394	A
1	AA	1398	A
1	AA	1413	A
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1452	C
1	AA	1492	A
1	AA	1494	G
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1505	G
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G

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Mol	Chain	Res	Type
1	AA	1530	G
1	AA	1533	C
1	AA	1535	C
1	AA	1536	C
23	AW	8	4SU
23	AW	14	A
23	AW	19	G
23	AW	20	U
23	AW	21	A
23	AW	45	G
23	AW	46	7MG
23	AW	48	C
23	AW	49	G
23	AW	59	A
23	AW	61	C
23	AW	68	G
23	AW	74	C
24	AX	19	U
24	AX	21	A
24	AX	47	U
24	AX	67	C
24	AX	68	G
24	AX	76	A
25	AY	5	G
25	AY	14	A
25	AY	19	G
25	AY	20	G
25	AY	21	A
25	AY	23	A
25	AY	45	G
25	AY	46	7MG
25	AY	47	U
25	AY	48	C
25	AY	54	5MU
25	AY	59	U
25	AY	60	C
26	BA	10	A
26	BA	14	A
26	BA	34	U
26	BA	42	A
26	BA	46	G
26	BA	63	A

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Mol	Chain	Res	Type
26	BA	71	A
26	BA	74	A
26	BA	75	G
26	BA	80	G
26	BA	83	A
26	BA	84	A
26	BA	98	G
26	BA	101	A
26	BA	118	A
26	BA	119	A
26	BA	120	U
26	BA	138	U
26	BA	139	U
26	BA	140	C
26	BA	141	G
26	BA	142	A
26	BA	162	U
26	BA	165	A
26	BA	181	A
26	BA	196	A
26	BA	199	A
26	BA	216	A
26	BA	222	A
26	BA	223	A
26	BA	233	A
26	BA	248	G
26	BA	249	C
26	BA	255	A
26	BA	265	A
26	BA	266	G
26	BA	271	G
26	BA	272	A
26	BA	276	U
26	BA	278	A
26	BA	279	A
26	BA	285	G
26	BA	294	A
26	BA	311	A
26	BA	321	U
26	BA	322	A
26	BA	324	A
26	BA	329	G

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Mol	Chain	Res	Type
26	BA	330	A
26	BA	361	G
26	BA	367	G
26	BA	371	A
26	BA	372	G
26	BA	386	G
26	BA	396	G
26	BA	404	A
26	BA	405	U
26	BA	411	G
26	BA	412	A
26	BA	424	G
26	BA	451	U
26	BA	455	C
26	BA	457	A
26	BA	467	G
26	BA	479	A
26	BA	480	A
26	BA	481	G
26	BA	490	C
26	BA	491	G
26	BA	504	A
26	BA	505	A
26	BA	508	A
26	BA	528	A
26	BA	531	C
26	BA	532	A
26	BA	533	G
26	BA	543	G
26	BA	544	C
26	BA	546	U
26	BA	547	A
26	BA	548	G
26	BA	549	G
26	BA	563	A
26	BA	572	A
26	BA	573	U
26	BA	574	A
26	BA	575	A
26	BA	586	A
26	BA	603	A
26	BA	613	A

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Mol	Chain	Res	Type
26	BA	627	A
26	BA	631	A
26	BA	637	A
26	BA	647	G
26	BA	654	A
26	BA	685	A
26	BA	686	U
26	BA	695	G
26	BA	717	C
26	BA	727	A
26	BA	730	A
26	BA	747	U
26	BA	751	A
26	BA	764	A
26	BA	775	G
26	BA	776	G
26	BA	781	A
26	BA	782	A
26	BA	784	G
26	BA	785	G
26	BA	789	A
26	BA	792	A
26	BA	802	A
26	BA	805	G
26	BA	812	C
26	BA	819	A
26	BA	827	U
26	BA	828	U
26	BA	830	G
26	BA	844	A
26	BA	845	A
26	BA	846	U
26	BA	858	G
26	BA	878	A
26	BA	896	A
26	BA	897	C
26	BA	910	A
26	BA	914	G
26	BA	915	C
26	BA	941	A
26	BA	946	C
26	BA	953	G

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Mol	Chain	Res	Type
26	BA	959	A
26	BA	961	C
26	BA	974	G
26	BA	983	A
26	BA	995	C
26	BA	996	A
26	BA	1009	A
26	BA	1012	U
26	BA	1013	C
26	BA	1021	A
26	BA	1022	G
26	BA	1026	G
26	BA	1033	U
26	BA	1040	A
26	BA	1046	A
26	BA	1047	G
26	BA	1060	U
26	BA	1061	U
26	BA	1065	U
26	BA	1066	U
26	BA	1068	G
26	BA	1070	A
26	BA	1071	G
26	BA	1072	C
26	BA	1077	A
26	BA	1088	A
26	BA	1089	A
26	BA	1090	A
26	BA	1092	C
26	BA	1094	U
26	BA	1098	A
26	BA	1111	A
26	BA	1112	G
26	BA	1132	U
26	BA	1133	A
26	BA	1135	C
26	BA	1136	G
26	BA	1143	A
26	BA	1151	A
26	BA	1175	A
26	BA	1176	U
26	BA	1178	C

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Mol	Chain	Res	Type
26	BA	1180	U
26	BA	1186	G
26	BA	1195	G
26	BA	1204	A
26	BA	1206	G
26	BA	1212	G
26	BA	1238	G
26	BA	1250	G
26	BA	1253	A
26	BA	1256	G
26	BA	1266	G
26	BA	1271	G
26	BA	1272	A
26	BA	1300	G
26	BA	1301	A
26	BA	1302	A
26	BA	1314	C
26	BA	1355	G
26	BA	1365	A
26	BA	1368	G
26	BA	1378	A
26	BA	1379	U
26	BA	1383	A
26	BA	1384	A
26	BA	1386	C
26	BA	1387	A
26	BA	1391	U
26	BA	1395	A
26	BA	1403	A
26	BA	1416	G
26	BA	1419	A
26	BA	1420	A
26	BA	1428	C
26	BA	1452	G
26	BA	1458	U
26	BA	1478	G
26	BA	1482	G
26	BA	1493	C
26	BA	1494	A
26	BA	1504	A
26	BA	1509	A
26	BA	1510	G

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Mol	Chain	Res	Type
26	BA	1515	A
26	BA	1533	C
26	BA	1535	A
26	BA	1536	C
26	BA	1537	G
26	BA	1560	G
26	BA	1566	A
26	BA	1569	A
26	BA	1578	U
26	BA	1581	G
26	BA	1583	A
26	BA	1584	U
26	BA	1585	C
26	BA	1607	C
26	BA	1610	A
26	BA	1616	A
26	BA	1646	C
26	BA	1647	U
26	BA	1648	U
26	BA	1652	A
26	BA	1664	A
26	BA	1674	G
26	BA	1694	C
26	BA	1715	G
26	BA	1729	U
26	BA	1730	C
26	BA	1732	C
26	BA	1738	G
26	BA	1757	A
26	BA	1758	U
26	BA	1764	C
26	BA	1773	A
26	BA	1784	A
26	BA	1785	A
26	BA	1791	A
26	BA	1800	C
26	BA	1801	A
26	BA	1802	A
26	BA	1808	A
26	BA	1816	C
26	BA	1819	A
26	BA	1829	A

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Mol	Chain	Res	Type
26	BA	1833	C
26	BA	1847	A
26	BA	1848	A
26	BA	1858	A
26	BA	1870	C
26	BA	1871	A
26	BA	1872	A
26	BA	1873	G
26	BA	1876	A
26	BA	1906	G
26	BA	1913	A
26	BA	1914	C
26	BA	1919	A
26	BA	1927	A
26	BA	1929	G
26	BA	1930	G
26	BA	1937	A
26	BA	1955	U
26	BA	1967	C
26	BA	1970	A
26	BA	1972	G
26	BA	1991	U
26	BA	1993	U
26	BA	1997	C
26	BA	2020	A
26	BA	2022	U
26	BA	2023	C
26	BA	2030	A
26	BA	2031	A
26	BA	2033	A
26	BA	2043	C
26	BA	2049	G
26	BA	2055	C
26	BA	2056	G
26	BA	2060	A
26	BA	2061	G
26	BA	2062	A
26	BA	2069	G
26	BA	2072	C
26	BA	2080	A
26	BA	2092	U
26	BA	2093	G

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Mol	Chain	Res	Type
26	BA	2095	A
26	BA	2097	A
26	BA	2110	G
26	BA	2111	U
26	BA	2112	G
26	BA	2114	A
26	BA	2116	G
26	BA	2117	A
26	BA	2118	U
26	BA	2119	A
26	BA	2126	A
26	BA	2127	G
26	BA	2128	G
26	BA	2131	U
26	BA	2132	U
26	BA	2133	G
26	BA	2135	A
26	BA	2147	A
26	BA	2158	A
26	BA	2162	G
26	BA	2163	A
26	BA	2164	C
26	BA	2169	A
26	BA	2170	A
26	BA	2171	A
26	BA	2172	U
26	BA	2173	A
26	BA	2189	U
26	BA	2190	G
26	BA	2194	U
26	BA	2198	A
26	BA	2199	A
26	BA	2204	G
26	BA	2211	A
26	BA	2212	A
26	BA	2214	C
26	BA	2225	A
26	BA	2226	C
26	BA	2238	G
26	BA	2239	G
26	BA	2243	U
26	BA	2246	G

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Mol	Chain	Res	Type
26	BA	2278	A
26	BA	2280	G
26	BA	2283	C
26	BA	2287	A
26	BA	2288	A
26	BA	2297	A
26	BA	2305	U
26	BA	2309	A
26	BA	2311	A
26	BA	2312	U
26	BA	2322	A
26	BA	2333	A
26	BA	2345	G
26	BA	2347	C
26	BA	2350	C
26	BA	2361	G
26	BA	2383	G
26	BA	2385	C
26	BA	2402	U
26	BA	2406	A
26	BA	2407	A
26	BA	2423	U
26	BA	2425	A
26	BA	2426	A
26	BA	2429	G
26	BA	2430	A
26	BA	2431	U
26	BA	2435	A
26	BA	2441	U
26	BA	2448	A
26	BA	2476	A
26	BA	2491	U
26	BA	2498	C
26	BA	2502	G
26	BA	2503	A
26	BA	2505	G
26	BA	2506	U
26	BA	2507	C
26	BA	2513	A
26	BA	2518	A
26	BA	2529	G
26	BA	2547	A

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Mol	Chain	Res	Type
26	BA	2550	G
26	BA	2554	U
26	BA	2566	A
26	BA	2567	G
26	BA	2572	A
26	BA	2573	C
26	BA	2602	A
26	BA	2609	U
26	BA	2613	U
26	BA	2615	U
26	BA	2629	U
26	BA	2630	G
26	BA	2636	C
26	BA	2689	U
26	BA	2690	U
26	BA	2714	G
26	BA	2716	C
26	BA	2718	G
26	BA	2726	A
26	BA	2729	G
26	BA	2733	A
26	BA	2744	G
26	BA	2748	A
26	BA	2757	A
26	BA	2765	A
26	BA	2778	A
26	BA	2782	G
26	BA	2791	G
26	BA	2809	A
26	BA	2818	U
26	BA	2820	A
26	BA	2823	A
26	BA	2836	U
26	BA	2867	G
26	BA	2872	A
26	BA	2873	A
26	BA	2879	A
26	BA	2880	C
26	BA	2886	A
26	BA	2887	A
26	BA	2903	U
27	BB	15	A

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Mol	Chain	Res	Type
27	BB	24	G
27	BB	41	G
27	BB	44	G
27	BB	53	A
27	BB	56	G
27	BB	66	A
27	BB	73	A
27	BB	88	C
27	BB	89	U
27	BB	90	C
27	BB	99	A
27	BB	109	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	96	U
1	AA	115	G
1	AA	1201	A
1	AA	1211	U
23	AW	13	C
25	AY	58	A
26	BA	271	G
26	BA	404	A
26	BA	479	A
26	BA	1606	C
26	BA	1913	A
26	BA	2109	U
26	BA	2146	C
26	BA	2225	A
26	BA	2506	U
26	BA	2756	U

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

21 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	$\#\|Z\| > 2$
23	T6A	AW	37	23	27,34,35	1.25	4 (14%)	29,49,52	1.43	4 (13%)
23	PSU	AW	39	23	18,21,22	1.30	3 (16%)	22,30,33	1.62	4 (18%)
24	4SU	AX	8	24	18,21,22	1.09	2 (11%)	26,30,33	0.82	2 (7%)
23	PSU	AW	55	23	18,21,22	1.30	3 (16%)	22,30,33	1.63	4 (18%)
25	PSU	AY	55	25	18,21,22	1.29	3 (16%)	22,30,33	1.62	4 (18%)
23	5MU	AW	54	23	19,22,23	0.92	2 (10%)	28,32,35	1.13	2 (7%)
23	3AU	AW	47	23	25,28,29	1.08	1 (4%)	32,40,43	0.93	2 (6%)
24	2MA	AX	37	24	17,25,26	0.95	1 (5%)	17,37,40	0.93	1 (5%)
23	4SU	AW	8	23	18,21,22	1.08	2 (11%)	26,30,33	0.82	2 (7%)
25	5MU	AY	54	25	19,22,23	0.94	2 (10%)	28,32,35	1.14	2 (7%)
24	PSU	AX	55	24	18,21,22	1.30	3 (16%)	22,30,33	1.61	4 (18%)
23	U8U	AW	34	22,23	19,24,25	0.88	1 (5%)	23,34,37	1.23	4 (17%)
23	7MG	AW	46	23	22,26,27	2.01	3 (13%)	29,39,42	1.22	4 (13%)
24	7MG	AX	46	24	22,26,27	2.05	3 (13%)	29,39,42	1.22	4 (13%)
25	6MZ	AY	37	25	18,25,26	1.25	3 (16%)	16,36,39	0.88	0
25	4SU	AY	8	25	18,21,22	1.08	2 (11%)	26,30,33	0.83	2 (7%)
24	5MU	AX	54	24	19,22,23	0.92	2 (10%)	28,32,35	1.13	2 (7%)
25	7MG	AY	46	25	22,26,27	2.05	3 (13%)	29,39,42	1.22	4 (13%)
24	QUO	AX	34	22,24	29,35,36	1.32	4 (13%)	31,52,55	1.47	7 (22%)
25	CM0	AY	34	25	22,26,27	0.96	1 (4%)	28,37,40	1.27	3 (10%)
24	PSU	AX	65	24	18,21,22	1.26	3 (16%)	22,30,33	1.55	5 (22%)

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
23	T6A	AW	37	23	-	0/19/41/42	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
25	PSU	AY	55	25	-	0/7/25/26	0/2/2/2
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
23	3AU	AW	47	23	-	6/16/34/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	2MA	AX	37	24	-	0/3/25/26	0/3/3/3
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
25	5MU	AY	54	25	-	2/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
23	U8U	AW	34	22,23	-	2/9/28/29	0/2/2/2
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3
24	7MG	AX	46	24	-	0/7/37/38	0/3/3/3
25	6MZ	AY	37	25	-	1/5/27/28	0/3/3/3
25	4SU	AY	8	25	-	0/7/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
25	7MG	AY	46	25	-	2/7/37/38	0/3/3/3
24	QUO	AX	34	22,24	-	2/6/43/44	0/4/4/4
25	CM0	AY	34	25	-	3/12/30/31	0/2/2/2
24	PSU	AX	65	24	-	4/7/25/26	0/2/2/2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	46	7MG	C8-N9	6.25	1.49	1.46
25	AY	46	7MG	C8-N9	6.23	1.49	1.46
23	AW	46	7MG	C8-N9	6.03	1.49	1.46
25	AY	46	7MG	C5-N7	5.84	1.42	1.35
24	AX	46	7MG	C5-N7	5.74	1.42	1.35
23	AW	46	7MG	C5-N7	5.70	1.42	1.35
24	AX	34	QUO	C6-N1	3.97	1.43	1.37
23	AW	47	3AU	C2-N1	3.58	1.43	1.38
24	AX	55	PSU	C2-N1	3.46	1.41	1.36
23	AW	55	PSU	C2-N1	3.44	1.41	1.36
25	AY	55	PSU	C2-N1	3.43	1.41	1.36
23	AW	39	PSU	C2-N1	3.41	1.41	1.36
24	AX	8	4SU	C4-S4	-3.22	1.62	1.68
23	AW	8	4SU	C4-S4	-3.20	1.62	1.68
23	AW	37	T6A	C10-N6	3.19	1.44	1.37
24	AX	37	2MA	C6-N1	3.19	1.45	1.38
25	AY	8	4SU	C4-S4	-3.16	1.62	1.68
24	AX	65	PSU	C2-N1	3.06	1.40	1.36
24	AX	65	PSU	C4-N3	2.69	1.43	1.38
25	AY	54	5MU	C2-N1	2.61	1.42	1.38
23	AW	55	PSU	C4-N3	2.60	1.43	1.38
25	AY	37	6MZ	C6-N1	2.60	1.37	1.34
23	AW	39	PSU	C4-N3	2.58	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AY	55	PSU	C4-N3	2.54	1.43	1.38
24	AX	55	PSU	C4-N3	2.54	1.43	1.38
24	AX	46	7MG	C6-N1	2.54	1.43	1.38
23	AW	37	T6A	C6-N1	2.51	1.37	1.34
25	AY	46	7MG	C6-N1	2.49	1.43	1.38
23	AW	46	7MG	C6-N1	2.47	1.43	1.38
23	AW	34	U8U	C4-N3	2.47	1.43	1.38
23	AW	54	5MU	C2-N1	2.44	1.42	1.38
24	AX	54	5MU	C2-N1	2.43	1.42	1.38
25	AY	34	CM0	C4-N3	2.36	1.43	1.38
25	AY	37	6MZ	C6-N6	2.34	1.38	1.35
24	AX	34	QUO	C5-C6	-2.33	1.42	1.47
25	AY	8	4SU	C2-N3	2.32	1.42	1.38
25	AY	37	6MZ	C2-N1	2.31	1.38	1.33
24	AX	55	PSU	C6-N1	2.29	1.40	1.36
24	AX	8	4SU	C2-N3	2.29	1.42	1.38
23	AW	55	PSU	C6-N1	2.28	1.40	1.36
23	AW	37	T6A	C12-C13	2.28	1.56	1.52
23	AW	8	4SU	C2-N3	2.25	1.42	1.38
23	AW	39	PSU	C6-N1	2.24	1.39	1.36
24	AX	34	QUO	C2-N2	2.23	1.39	1.34
24	AX	54	5MU	C2-N3	2.22	1.41	1.38
23	AW	37	T6A	C2-N3	2.22	1.35	1.32
23	AW	54	5MU	C2-N3	2.22	1.41	1.38
25	AY	54	5MU	C2-N3	2.20	1.41	1.38
25	AY	55	PSU	C6-N1	2.20	1.39	1.36
24	AX	65	PSU	C6-N1	2.13	1.39	1.36
24	AX	34	QUO	C13-C12	2.08	1.55	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	55	PSU	C6-C5-C4	5.07	121.74	118.20
24	AX	55	PSU	C6-C5-C4	4.99	121.69	118.20
23	AW	39	PSU	C6-C5-C4	4.96	121.67	118.20
25	AY	55	PSU	C6-C5-C4	4.94	121.65	118.20
23	AW	37	T6A	C12-N11-C10	-4.44	114.53	121.94
24	AX	65	PSU	C6-C5-C4	4.18	121.12	118.20
25	AY	34	CM0	C7-O5-C5	-4.15	112.14	117.58
24	AX	34	QUO	O6-C6-N1	-3.51	116.50	120.65
23	AW	34	U8U	C1'-N1-C6	-3.35	115.55	121.12
24	AX	54	5MU	C4-N3-C2	-3.15	123.27	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	54	5MU	C4-N3-C2	-3.12	123.31	127.35
25	AY	54	5MU	C4-N3-C2	-3.12	123.31	127.35
25	AY	54	5MU	C6-C5-C4	2.97	120.51	118.03
23	AW	54	5MU	C6-C5-C4	2.94	120.49	118.03
24	AX	54	5MU	C6-C5-C4	2.93	120.48	118.03
24	AX	34	QUO	O6-C6-C5	2.93	130.11	123.98
24	AX	46	7MG	C5-C4-N9	2.85	110.04	106.35
25	AY	46	7MG	C5-C4-N9	2.83	110.02	106.35
23	AW	46	7MG	C5-C4-N9	2.78	109.96	106.35
24	AX	65	PSU	O2-C2-N1	-2.73	119.79	122.79
25	AY	55	PSU	O2-C2-N1	-2.72	119.79	122.79
25	AY	8	4SU	C4-N3-C2	-2.71	124.71	127.34
23	AW	39	PSU	O2-C2-N1	-2.70	119.82	122.79
25	AY	34	CM0	C4-N3-C2	-2.69	123.87	127.35
24	AX	34	QUO	C10-N11-C12	-2.68	109.26	114.90
24	AX	37	2MA	N1-C2-N3	2.66	127.46	123.06
23	AW	8	4SU	C4-N3-C2	-2.65	124.76	127.34
23	AW	55	PSU	O2-C2-N1	-2.65	119.87	122.79
24	AX	8	4SU	C4-N3-C2	-2.65	124.77	127.34
24	AX	55	PSU	O2-C2-N1	-2.62	119.90	122.79
23	AW	47	3AU	C1'-N1-C2	2.57	121.33	116.99
24	AX	34	QUO	C16-C12-C13	2.46	106.83	103.18
24	AX	34	QUO	O13-C13-C12	-2.44	106.39	112.92
24	AX	65	PSU	O4-C4-N3	-2.38	115.55	120.12
23	AW	37	T6A	C4-C5-N7	2.35	111.85	109.40
24	AX	46	7MG	C2-N1-C6	-2.34	120.84	125.10
24	AX	34	QUO	C5-C6-N1	-2.34	113.38	115.36
23	AW	46	7MG	C2-N1-C6	-2.32	120.87	125.10
23	AW	46	7MG	C4-C5-N7	2.30	108.72	105.53
24	AX	46	7MG	O6-C6-N1	-2.28	115.75	120.12
23	AW	37	T6A	O14-C14-C12	2.28	113.70	109.13
25	AY	46	7MG	C2-N1-C6	-2.27	120.96	125.10
25	AY	46	7MG	C4-C5-N7	2.26	108.67	105.53
23	AW	46	7MG	O6-C6-N1	-2.24	115.82	120.12
24	AX	46	7MG	C4-C5-N7	2.24	108.64	105.53
25	AY	46	7MG	O6-C6-N1	-2.23	115.85	120.12
24	AX	65	PSU	O4-C4-C5	2.14	129.66	124.05
25	AY	8	4SU	C6-C5-C4	2.12	121.79	119.95
23	AW	47	3AU	C4-N3-C2	-2.09	122.00	124.63
24	AX	34	QUO	C2-N1-C6	-2.08	121.26	125.10
24	AX	8	4SU	C6-C5-C4	2.08	121.75	119.95
23	AW	34	U8U	C5-C6-N1	-2.06	120.14	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	8	4SU	C6-C5-C4	2.06	121.73	119.95
23	AW	55	PSU	N1-C2-N3	2.05	117.45	115.13
25	AY	55	PSU	N1-C2-N3	2.05	117.45	115.13
23	AW	37	T6A	N6-C6-N1	2.05	121.46	118.72
23	AW	34	U8U	O4-C4-C5	2.04	128.00	124.96
23	AW	34	U8U	C6-C5-C4	2.04	122.36	118.46
23	AW	39	PSU	N1-C2-N3	2.04	117.44	115.13
24	AX	65	PSU	N1-C2-N3	2.03	117.43	115.13
25	AY	34	CM0	O4-C4-N3	-2.03	116.23	120.12
24	AX	55	PSU	O4-C4-N3	-2.02	116.24	120.12
23	AW	39	PSU	O4-C4-N3	-2.02	116.25	120.12
25	AY	55	PSU	O4-C4-N3	-2.01	116.26	120.12
24	AX	55	PSU	N1-C2-N3	2.01	117.41	115.13
23	AW	55	PSU	O4-C4-N3	-2.01	116.27	120.12

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	34	U8U	C3'-C4'-C5'-O5'
23	AW	34	U8U	O4'-C4'-C5'-O5'
23	AW	46	7MG	C3'-C4'-C5'-O5'
23	AW	47	3AU	C10-C11-C12-N40
24	AX	34	QUO	C13-C12-N11-C10
24	AX	34	QUO	C16-C12-N11-C10
24	AX	65	PSU	C2'-C1'-C5-C4
24	AX	65	PSU	O4'-C1'-C5-C4
24	AX	65	PSU	O4'-C1'-C5-C6
25	AY	46	7MG	C4'-C5'-O5'-P
25	AY	46	7MG	C2'-C1'-N9-C8
25	AY	54	5MU	C3'-C4'-C5'-O5'
25	AY	54	5MU	O4'-C4'-C5'-O5'
25	AY	34	CM0	O5-C7-C8-O8
23	AW	46	7MG	O4'-C4'-C5'-O5'
23	AW	47	3AU	O4'-C4'-C5'-O5'
24	AX	65	PSU	C4'-C5'-O5'-P
23	AW	47	3AU	N40-C12-C13-O31
25	AY	34	CM0	O5-C7-C8-O9
23	AW	46	7MG	C4'-C5'-O5'-P
23	AW	47	3AU	C3'-C4'-C5'-O5'
23	AW	47	3AU	N40-C12-C13-O30
23	AW	47	3AU	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	AY	37	6MZ	C3'-C4'-C5'-O5'
25	AY	34	CM0	C6-C5-O5-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	AY	55	PSU	1	0
23	AW	34	U8U	1	0
25	AY	34	CM0	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
59	ERY	BA	9000	-	53,53,53	1.16	5 (9%)	82,82,82	1.69	23 (28%)
58	LYS	AW	101	23	7,8,9	0.81	0	3,8,10	0.76	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	ERY	BA	9000	-	-	13/72/107/107	0/3/3/3
58	LYS	AW	101	23	-	1/6/7/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	BA	9000	ERY	O13-C12	-2.82	1.39	1.44
59	BA	9000	ERY	O9-C26	-2.77	1.39	1.44
59	BA	9000	ERY	O10-C6	-2.64	1.40	1.44
59	BA	9000	ERY	O2-C13	-2.53	1.42	1.46
59	BA	9000	ERY	C23-C24	2.09	1.58	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	BA	9000	ERY	C36-C13-C12	-3.91	107.79	115.20
59	BA	9000	ERY	C34-C10-C11	-3.82	109.62	114.38
59	BA	9000	ERY	C12-C11-C10	-3.39	112.18	116.43
59	BA	9000	ERY	O13-C12-C13	3.29	112.56	107.28
59	BA	9000	ERY	O2-C1-C2	3.26	118.70	111.56
59	BA	9000	ERY	C16-C15-C14	-3.12	109.66	115.07
59	BA	9000	ERY	C20-O5-C16	-3.02	111.25	117.55
59	BA	9000	ERY	O2-C1-O1	-2.86	118.60	123.94
59	BA	9000	ERY	C22-O9-C26	-2.83	108.42	112.91
59	BA	9000	ERY	C35-C12-C13	-2.58	107.67	111.31
59	BA	9000	ERY	O5-C16-C17	2.54	107.58	103.81
59	BA	9000	ERY	O6-C17-C16	-2.50	106.45	111.12
59	BA	9000	ERY	O3-C3-C2	2.43	115.37	111.14
59	BA	9000	ERY	C27-C26-C25	-2.42	109.60	113.40
59	BA	9000	ERY	C6-C5-C4	-2.37	110.70	114.05
59	BA	9000	ERY	C7-C6-C5	-2.37	105.86	110.48
59	BA	9000	ERY	C22-O7-C5	-2.31	112.25	116.25
59	BA	9000	ERY	O8-C23-C24	-2.30	105.67	109.77
59	BA	9000	ERY	O5-C16-C15	-2.15	109.51	112.96
59	BA	9000	ERY	O7-C22-O9	-2.09	104.82	110.67
59	BA	9000	ERY	O4-C18-C21	2.08	111.20	106.70
59	BA	9000	ERY	C15-C16-C17	2.07	111.38	107.67
59	BA	9000	ERY	C25-C24-N1	-2.02	109.96	115.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AW	101	LYS	O-C-CA-CB
59	BA	9000	ERY	C34-C10-C11-C12
59	BA	9000	ERY	O13-C12-C13-O2
59	BA	9000	ERY	O13-C12-C13-C36

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Mol	Chain	Res	Type	Atoms
59	BA	9000	ERY	C35-C12-C13-O2
59	BA	9000	ERY	C35-C12-C13-C36
59	BA	9000	ERY	C11-C12-C13-O2
59	BA	9000	ERY	C11-C12-C13-C36
59	BA	9000	ERY	C34-C10-C11-O12
59	BA	9000	ERY	O2-C13-C36-C37
59	BA	9000	ERY	C9-C10-C11-O12
59	BA	9000	ERY	C9-C10-C11-C12
59	BA	9000	ERY	C25-C24-N1-C29
59	BA	9000	ERY	C12-C13-C36-C37

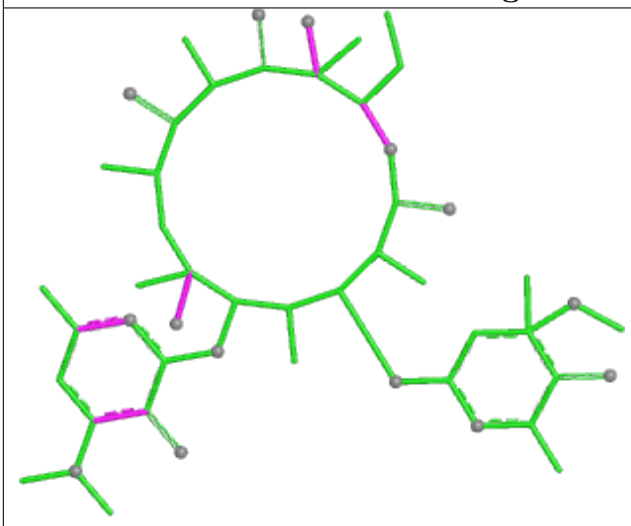
There are no ring outliers.

2 monomers are involved in 15 short contacts:

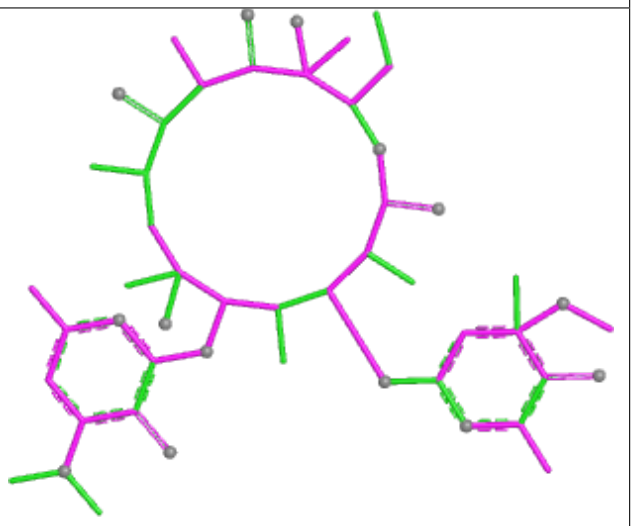
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	BA	9000	ERY	12	0
58	AW	101	LYS	3	0

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

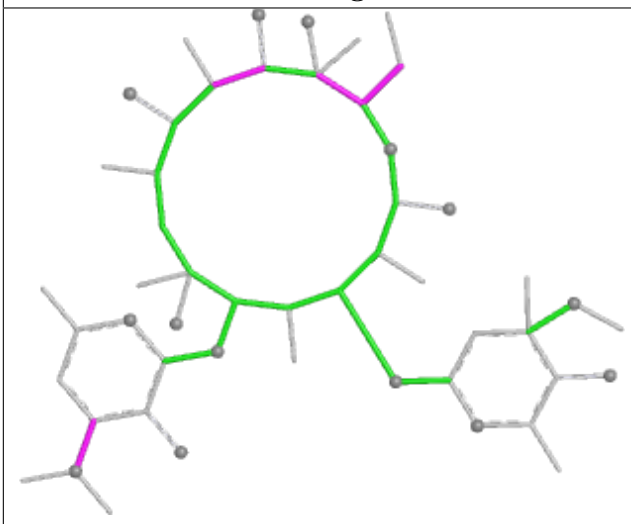
Ligand ERY BA 9000



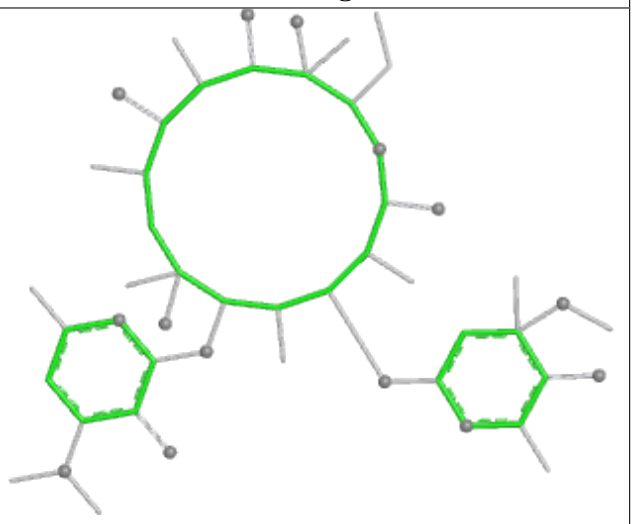
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	BA	1
23	AW	1
25	AY	1
1	AA	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	13.72
1	AW	15:G	O3'	18:G	P	9.77
1	AY	15:G	O3'	18:G	P	6.82
1	AA	99:C	O3'	100:G	P	4.17

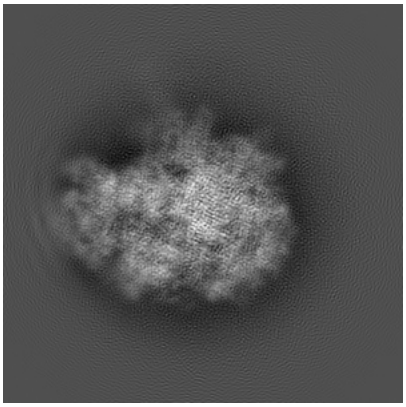
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8175. These allow visual inspection of the internal detail of the map and identification of artifacts.

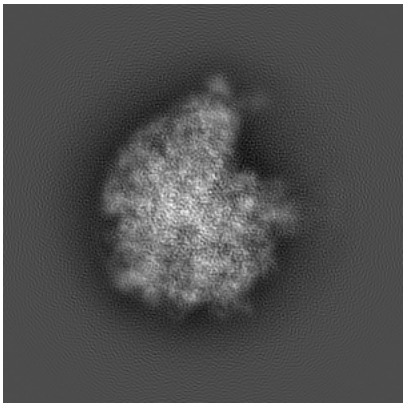
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

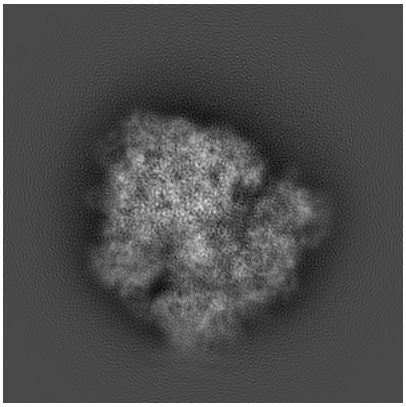
6.1.1 Primary map



X



Y

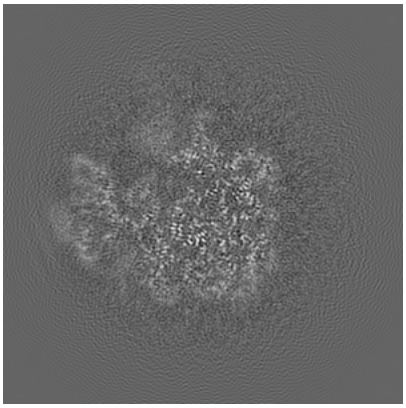


Z

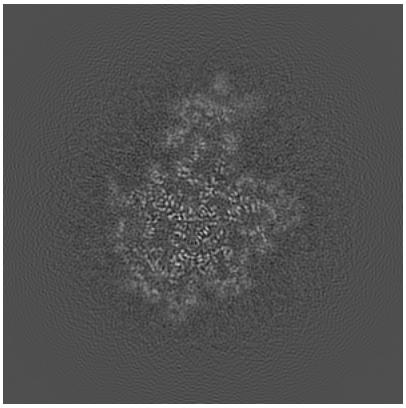
The images above show the map projected in three orthogonal directions.

6.2 Central slices

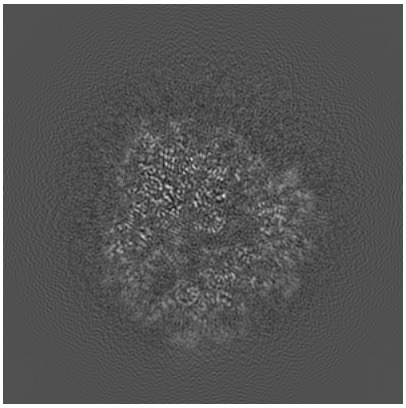
6.2.1 Primary map



X Index: 184



Y Index: 184

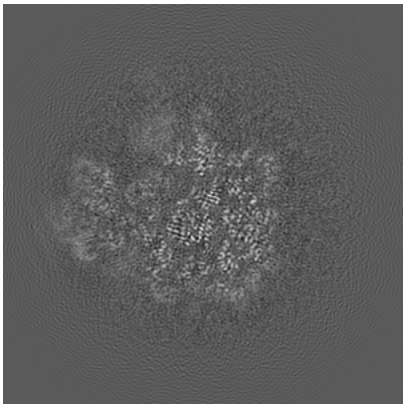


Z Index: 184

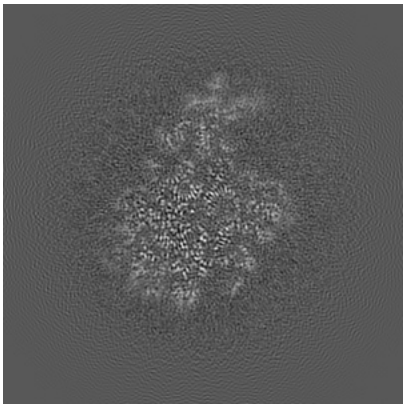
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

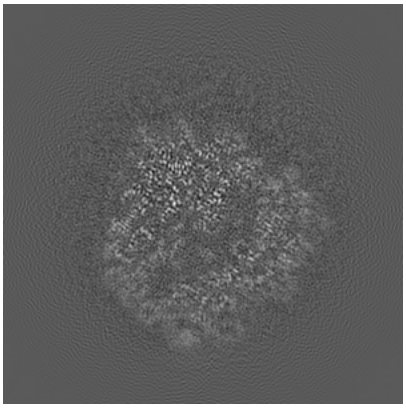
6.3.1 Primary map



X Index: 181



Y Index: 177



Z Index: 186

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 0.00194. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

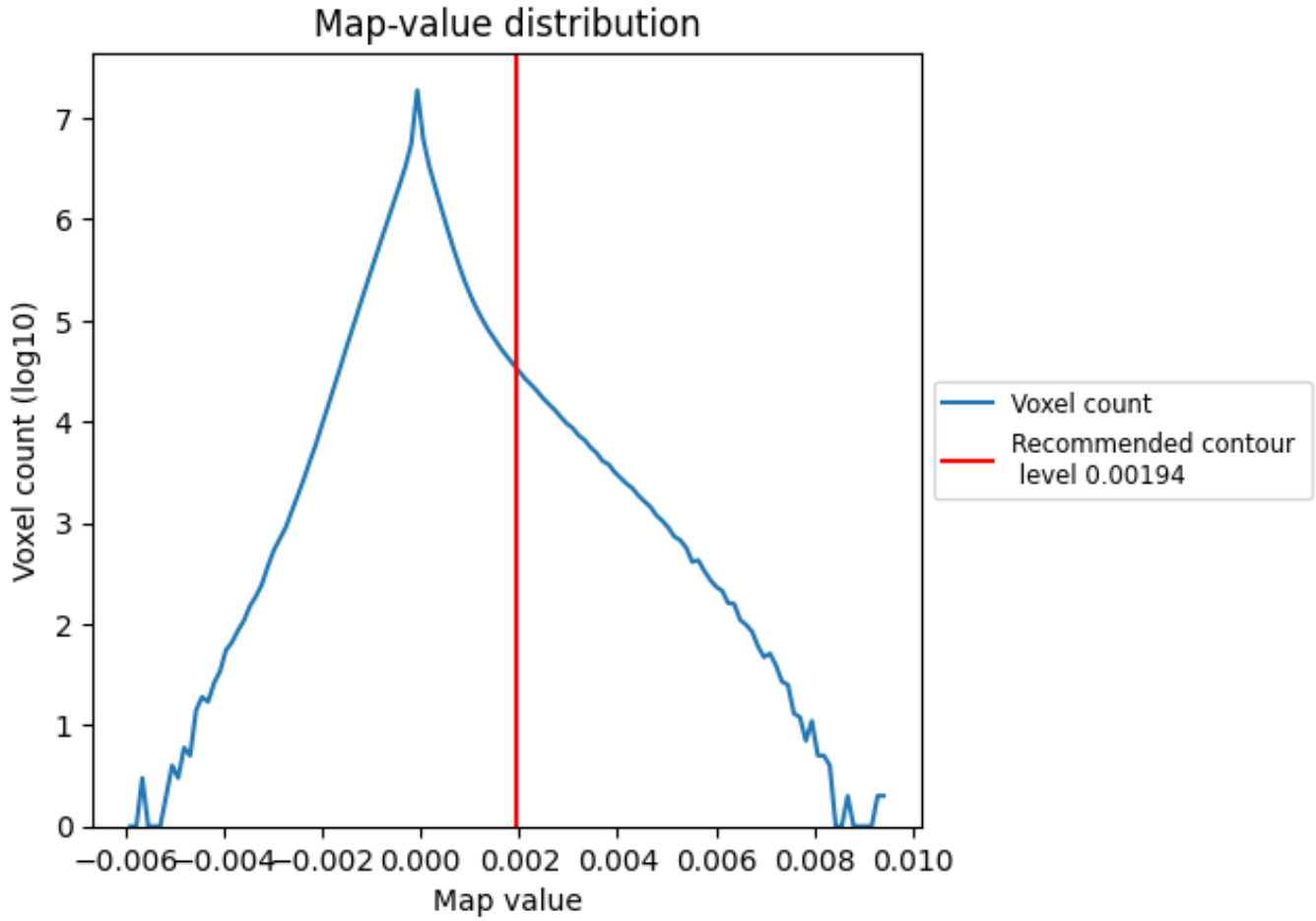
6.5 Mask visualisation (i)

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

7 Map analysis

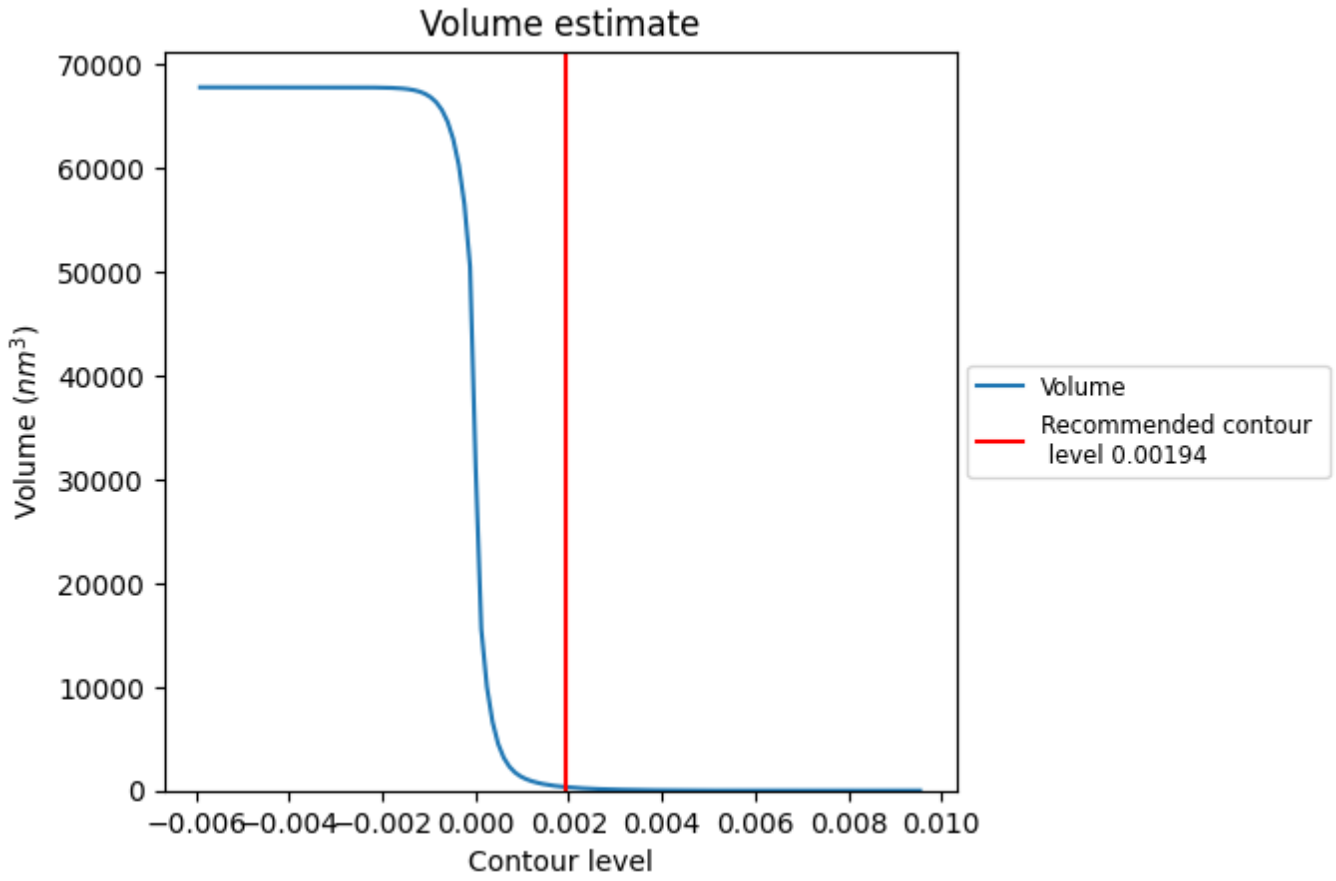
This section contains the results of statistical analysis of the map.

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.

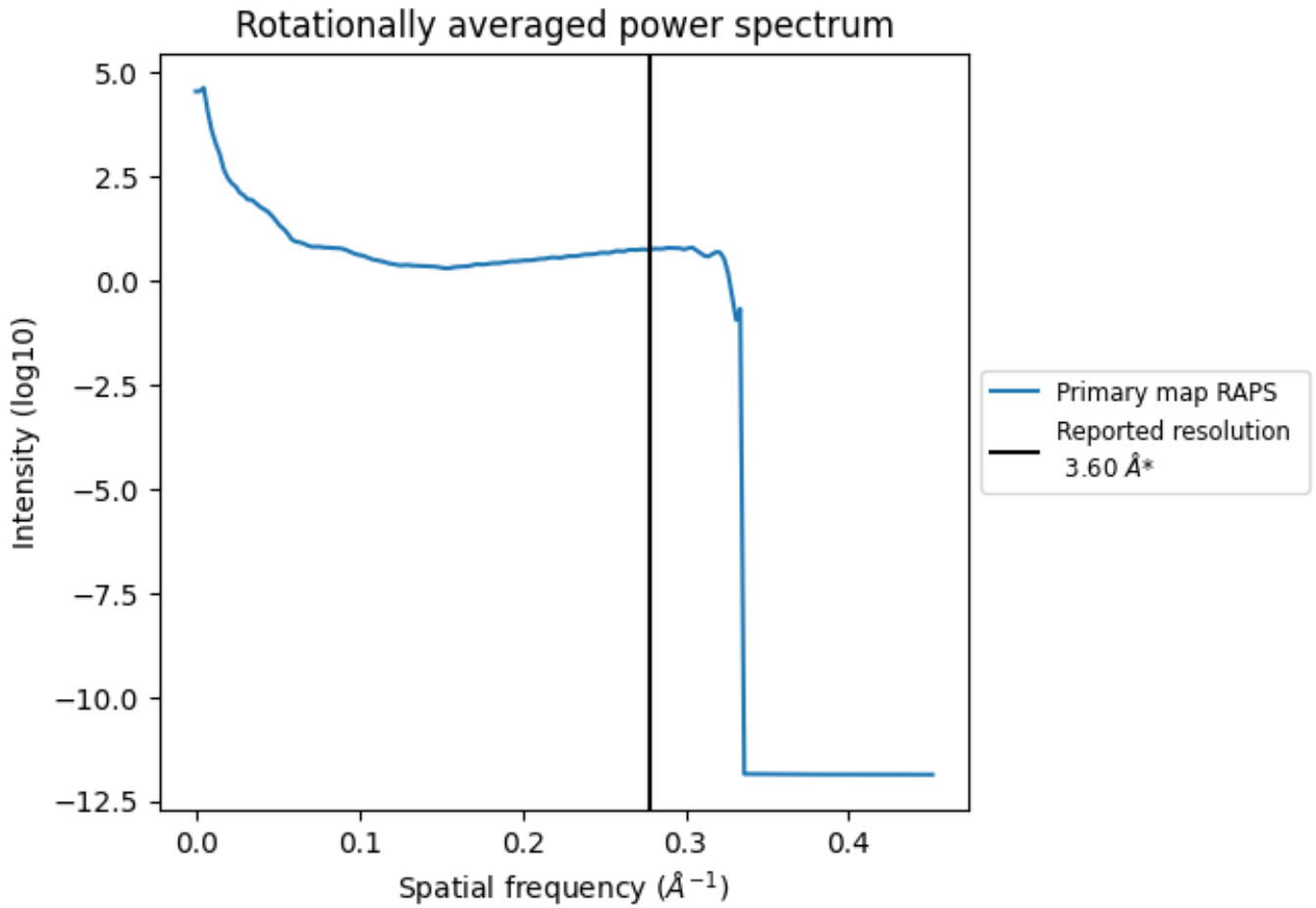
7.2 Volume estimate



The volume at the recommended contour level is 337 nm^3; this corresponds to an approximate mass of 305 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 0.278 $Å^{-1}$

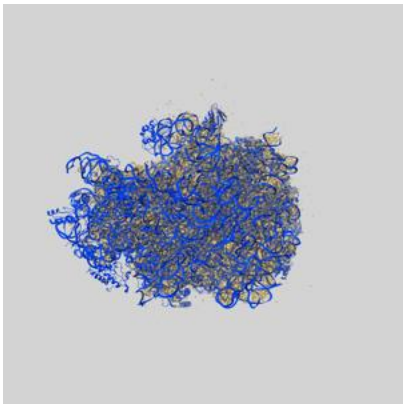
8 Fourier-Shell correlation

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

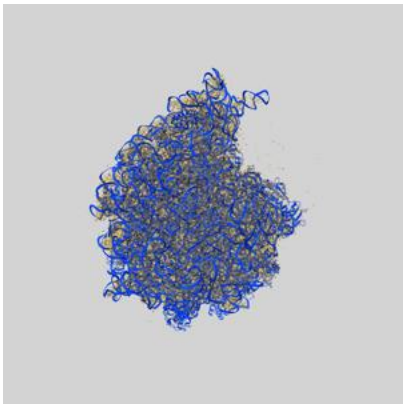
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8175 and PDB model 5JTE. Per-residue inclusion information can be found in section 3 on page 15.

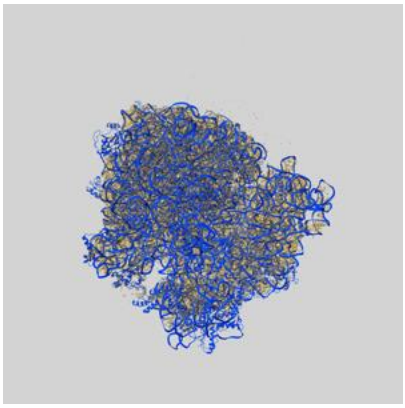
9.1 Map-model overlay



X



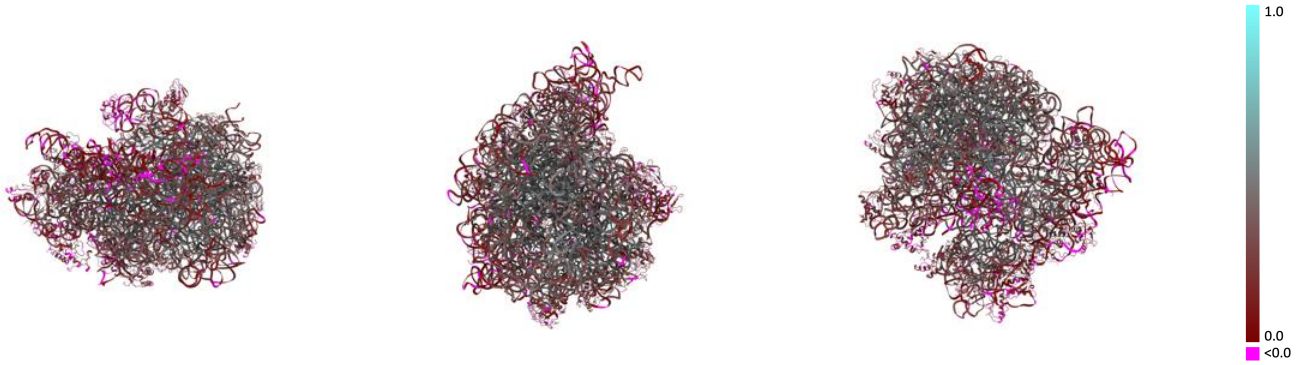
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

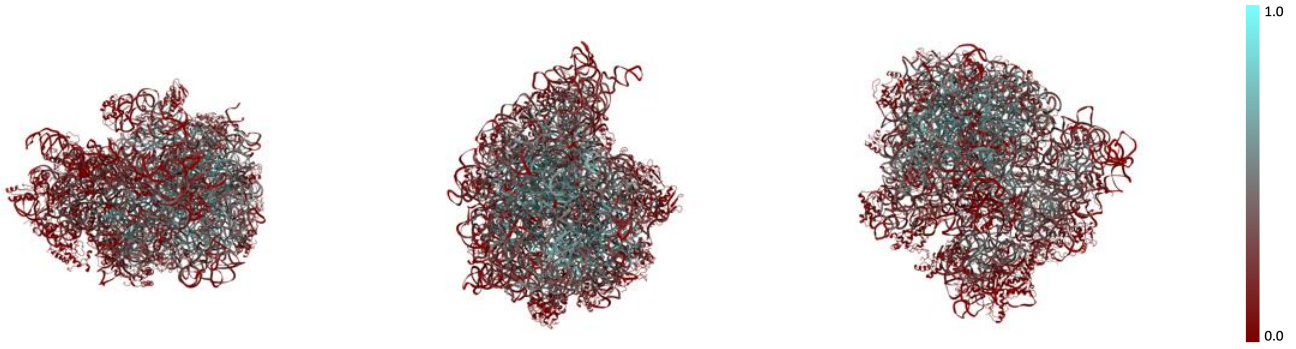
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

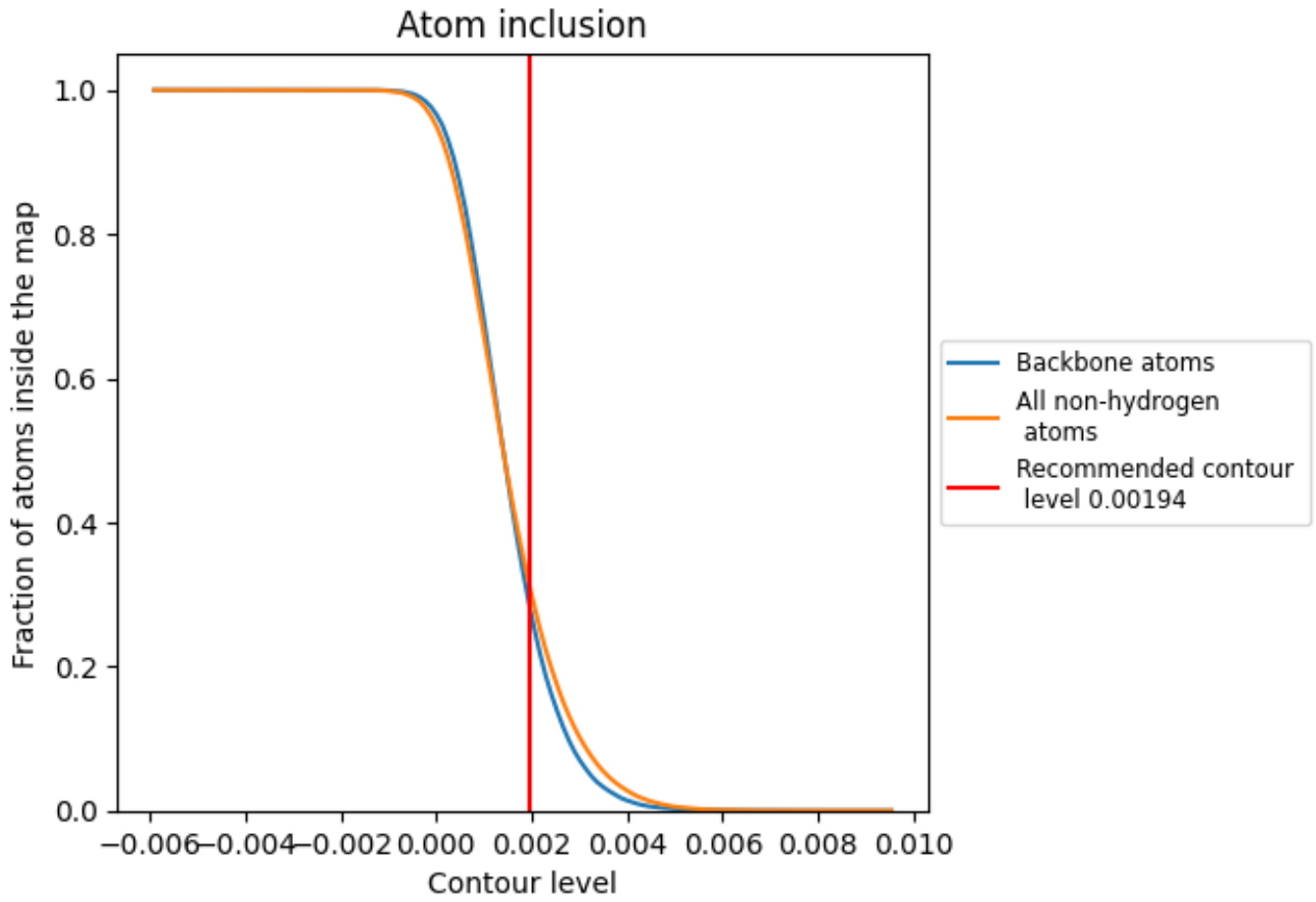
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00194).

9.4 Atom inclusion (i)



At the recommended contour level, 29% of all backbone atoms, 32% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3164	0.3150
AA	0.3038	0.2960
AB	0.0042	0.1140
AC	0.0526	0.2080
AD	0.0503	0.1960
AE	0.1163	0.2570
AF	0.0741	0.1890
AG	0.0358	0.2010
AH	0.1094	0.2610
AI	0.0225	0.1760
AJ	0.0250	0.1550
AK	0.1043	0.2310
AL	0.1976	0.2820
AM	0.0611	0.1920
AN	0.0834	0.2330
AO	0.1866	0.3100
AP	0.0813	0.1500
AQ	0.1551	0.2000
AR	0.1376	0.2600
AS	0.0725	0.2110
AT	0.1462	0.2250
AU	0.0222	0.1370
AV	0.4450	0.4210
AW	0.1273	0.1380
AX	0.2446	0.3190
AY	0.0807	0.1960
B0	0.2734	0.3400
B1	0.1022	0.3010
B2	0.3972	0.3760
B3	0.3279	0.3790
B4	0.2740	0.3260
B5	0.2361	0.3650
BA	0.4516	0.3820
BB	0.2720	0.2950
BC	0.3219	0.3360

Continued on next page...

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Chain	Atom inclusion	Q-score
BD	0.2711	0.3410
BE	0.1500	0.2550
BF	0.0503	0.1400
BG	0.0817	0.1870
BH	0.0112	0.0990
BI	0.0010	0.0320
BJ	0.2382	0.3250
BK	0.2662	0.3370
BL	0.2087	0.2950
BM	0.2697	0.3220
BN	0.3286	0.3430
BO	0.0579	0.2200
BP	0.2117	0.2850
BQ	0.3722	0.3620
BR	0.1819	0.2870
BS	0.2416	0.3220
BT	0.1537	0.2370
BU	0.0847	0.2060
BV	0.1558	0.2680
BW	0.2847	0.3480
BX	0.2263	0.3140
BY	0.1026	0.1930
BZ	0.2128	0.3060