



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:34 PM BST

PDB ID : 3J9W
EMDB ID: : EMD-6306
Title : Cryo-EM structure of the Bacillus subtilis MifM-stalled ribosome complex
Authors : Sohmen, D.; Chiba, S.; Shimokawa-Chiba, N.; Innis, C.A.; Berninghausen, O.; Beckmann, R.; Ito, K.; Wilson, D.N.
Deposited on : 2015-03-16
Resolution : 3.90 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

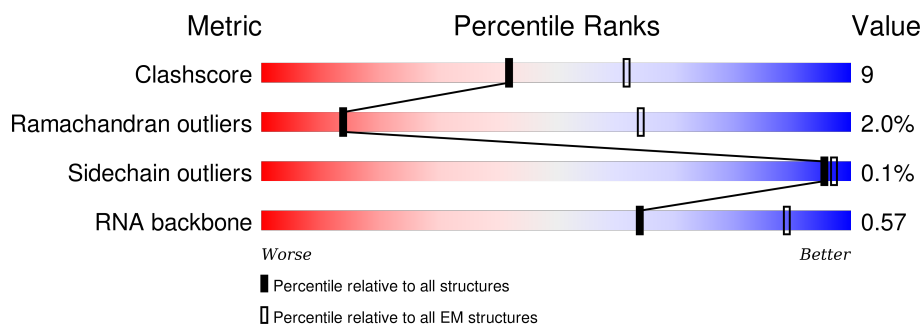
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.




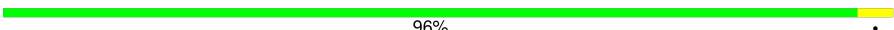








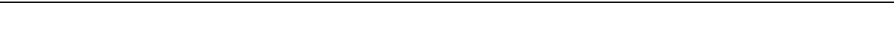

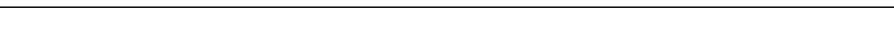
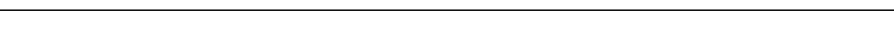











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	AA	1555	
2	AB	246	
3	AC	218	
4	AD	200	
5	AE	166	
6	AF	95	
7	AG	156	
8	AH	132	















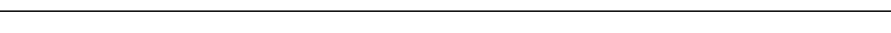
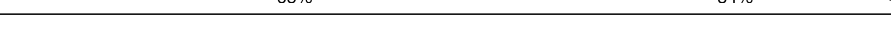





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Mol	Chain	Length	Quality of chain
9	AI	130	 93% 5% .
10	AJ	102	 96% .
11	AK	131	 85% 5% 10%
12	AL	138	 93% 7% .
13	AM	121	 89% 7% . .
14	AN	61	 90% 7% . .
15	AO	89	 97% . .
16	AP	90	 97% . .
17	AQ	87	 97% . .
18	AR	79	 85% . . 10%
19	AS	92	 87% . 9%
20	AT	88	 92% 6% .
21	AX	77	 57% 18% 22% .
22	AY	19	 11% 58% 32%
23	AZ	95	 15% 8% . 75%
24	B0	62	 56% 34% . 6%
25	B1	66	 71% 27% .
26	B2	59	 71% 27% .
27	B3	66	 70% 26% . .
28	B4	59	 66% 25% 8%
29	B5	49	 55% 43% .
30	B6	44	 80% 20%
31	B7	66	 47% 48% . .
32	B8	37	 84% 14% .
33	BA	2928	 44% 33% 18% 6%

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Mol	Chain	Length	Quality of chain
34	BB	119	
35	BD	277	
36	BE	209	
37	BF	207	
38	BG	179	
39	BH	179	
40	BJ	166	
41	BK	141	
42	BM	145	
43	BN	122	
44	BO	146	
45	BP	144	
46	BQ	120	
47	BR	120	
48	BS	115	
49	BT	119	
50	BU	102	
51	BV	113	
52	BW	95	
53	BX	103	
54	BZ	94	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 135425 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
1	AA	1544	Total	C	N	O	P	0	0
			33115	14768	6067	10736	1544		

- Molecule 2 is a protein called 30S ribosomal protein uS2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	AB	224	Total	C	N	O	0	0
			896	448	224	224		

- Molecule 3 is a protein called 30S ribosomal protein uS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	AC	210	Total	C	N	O	0	0
			840	420	210	210		

- Molecule 4 is a protein called 30S ribosomal protein uS4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	AD	199	Total	C	N	O	0	0
			797	398	199	200		

- Molecule 5 is a protein called 30S ribosomal protein uS5.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AE	165	Total	C	N	O	0	0
			661	330	165	166		

- Molecule 6 is a protein called 30S ribosomal protein bS6.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	AF	95	Total	C	N	O	0	0
			381	190	95	96		

- Molecule 7 is a protein called 30S ribosomal protein uS7.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AG	153	Total	C	N	O	0	0
			613	306	153	154		

- Molecule 8 is a protein called 30S ribosomal protein uS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AH	131	Total	C	N	O	0	0
			525	262	131	132		

- Molecule 9 is a protein called 30S ribosomal protein uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AI	130	Total	C	N	O	0	0
			521	260	130	131		

- Molecule 10 is a protein called 30S ribosomal protein uS10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	AJ	102	Total	C	N	O	0	0
			409	204	102	103		

- Molecule 11 is a protein called 30S ribosomal protein uS11.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	AK	118	Total	C	N	O	0	0
			472	236	118	118		

- Molecule 12 is a protein called 30S ribosomal protein uS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	AL	137	Total	C	N	O	0	0
			549	274	137	138		

- Molecule 13 is a protein called 30S ribosomal protein uS13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	AM	119	Total	C	N	O	0	0
			476	238	119	119		

- Molecule 14 is a protein called 30S ribosomal protein uS14.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	AN	60	Total	C	N	O	0	0
			241	120	60	61		

- Molecule 15 is a protein called 30S ribosomal protein uS15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	AO	88	Total	C	N	O	0	0
			353	176	88	89		

- Molecule 16 is a protein called 30S ribosomal protein bS16.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	AP	89	Total	C	N	O	0	0
			357	178	89	90		

- Molecule 17 is a protein called 30S ribosomal protein uS17.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	AQ	86	Total	C	N	O	0	0
			345	172	86	87		

- Molecule 18 is a protein called 30S ribosomal protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	71	Total	C	N	O	0	0
			285	142	71	72		

- Molecule 19 is a protein called 30S ribosomal protein uS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	AS	84	Total	C	N	O	0	0
			336	168	84	84		

- Molecule 20 is a protein called 30S ribosomal protein bS20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	AT	86	Total	C	N	O	0	0
			345	172	86	87		

- Molecule 21 is a RNA chain called tRNA-Asp.

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AY	19	Total	C	N	O	P	0	0
			415	185	82	129	19		

- Molecule 23 is a protein called MifM.

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

- Molecule 24 is a protein called 50S ribosomal protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B0	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 25 is a protein called 50S ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B1	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 26 is a protein called 50S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B2	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 27 is a protein called 50S ribosomal protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B3	64	Total	C	N	O	S	0	0
			503	314	92	92	5		

- Molecule 28 is a protein called 50S ribosomal protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B4	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 29 is a protein called 50S ribosomal protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B5	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 30 is a protein called 50S ribosomal protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B6	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 31 is a protein called 50S ribosomal protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B7	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 32 is a protein called 50S ribosomal protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B8	36	Total	C	N	O	S	0	0
			288	181	59	44	4		

- Molecule 33 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 34 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 35 is a protein called 50S ribosomal protein uL2.

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

- Molecule 36 is a protein called 50S ribosomal protein uL3.

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

- Molecule 37 is a protein called 50S ribosomal protein uL4.

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

- Molecule 38 is a protein called 50S ribosomal protein uL5.

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

- Molecule 39 is a protein called 50S ribosomal protein uL6.

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

- Molecule 40 is a protein called 50S ribosomal protein uL10.

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

- Molecule 41 is a protein called 50S ribosomal protein uL11.

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

- Molecule 42 is a protein called 50S ribosomal protein uL13.

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

- Molecule 43 is a protein called 50S ribosomal protein uL14.

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

- Molecule 44 is a protein called 50S ribosomal protein uL15.

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

- Molecule 45 is a protein called 50S ribosomal protein uL16.

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

- Molecule 46 is a protein called 50S ribosomal protein bL17.

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

- Molecule 47 is a protein called 50S ribosomal protein uL18.

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

- Molecule 48 is a protein called 50S ribosomal protein bL19.

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

- Molecule 49 is a protein called 50S ribosomal protein bL20.

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

- Molecule 50 is a protein called 50S ribosomal protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BU	101	Total	C	N	O	S	0	0
			786	501	139	146			

- Molecule 51 is a protein called 50S ribosomal protein uL22.

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

- Molecule 52 is a protein called 50S ribosomal protein uL23.

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

- Molecule 53 is a protein called 50S ribosomal protein uL24.

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

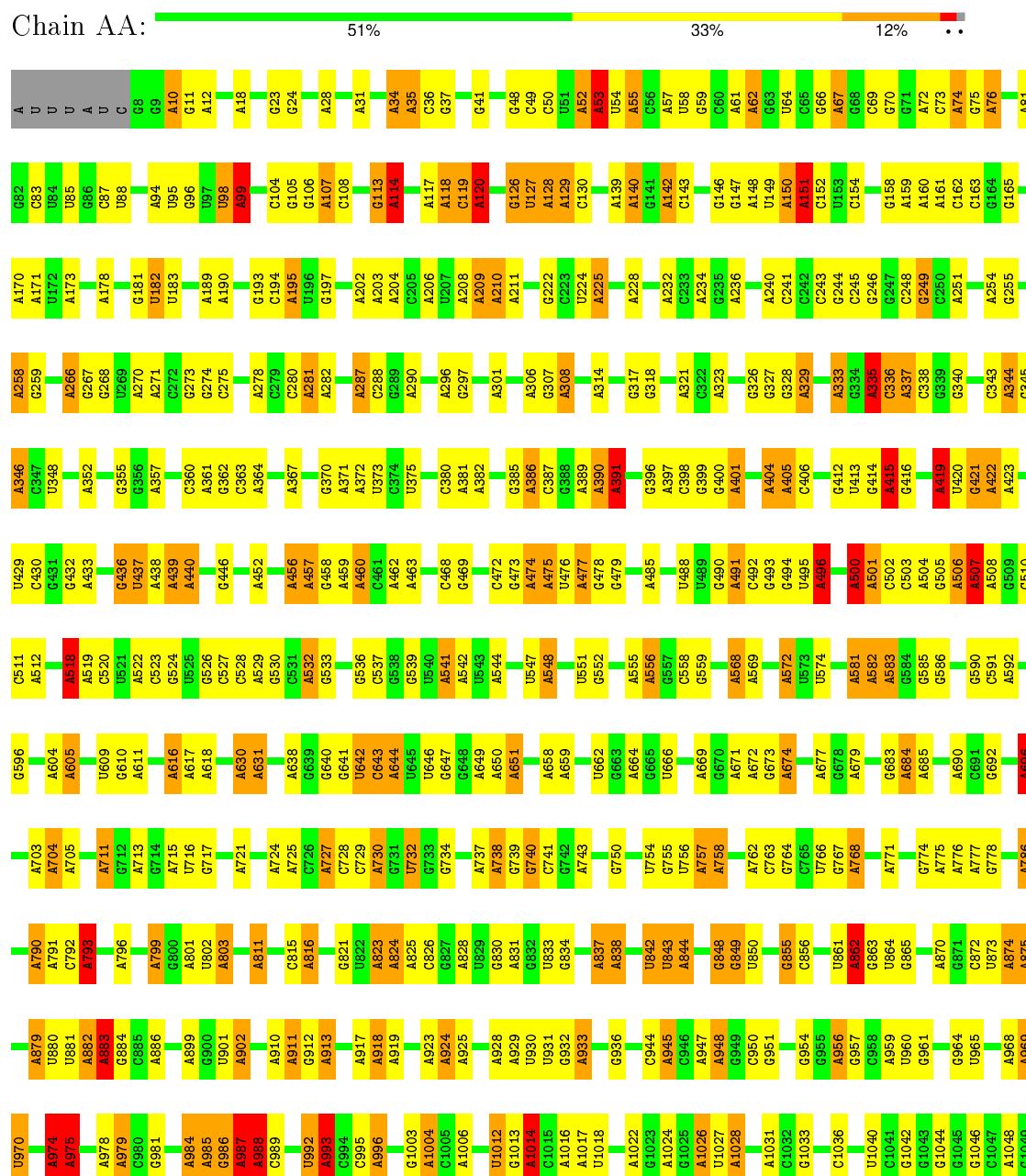
- Molecule 54 is a protein called 50S ribosomal protein bL27.

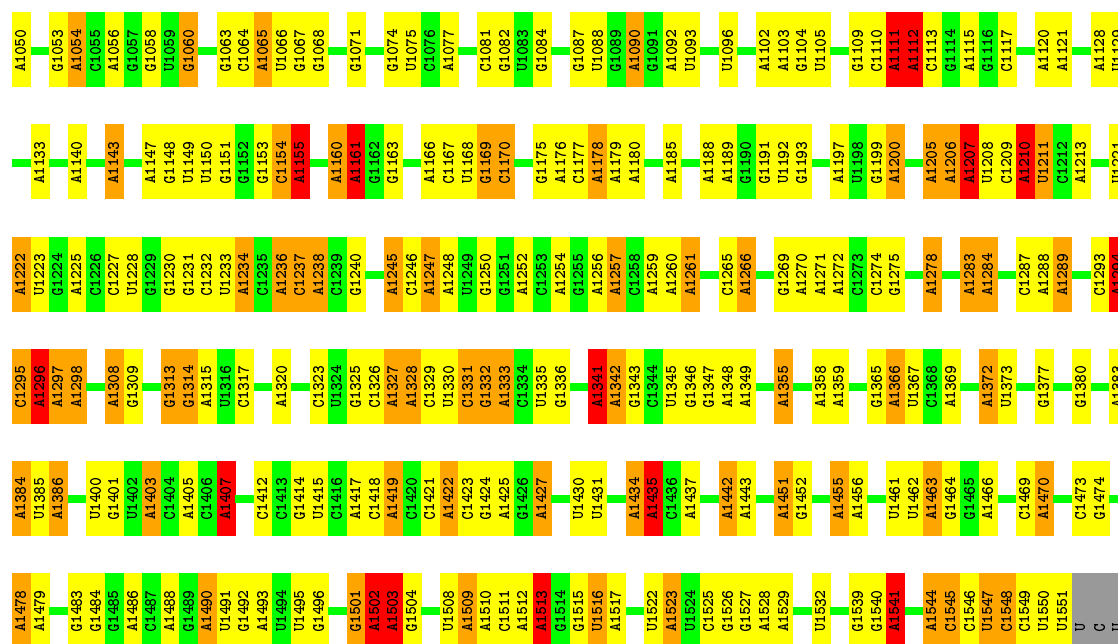
Mol	Chain	Residues	Atoms					AltConf	Trace
54	BZ	82	Total	C	N	O	S	0	0
			630	390	123	117			

3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA





A

- Molecule 2: 30S ribosomal protein uS2

Chain AB: 88% 9%



- Molecule 3: 30S ribosomal protein uS3

Chain AC: 94%



- Molecule 4: 30S ribosomal protein uS4

Chain AD: 97%



- Molecule 5: 30S ribosomal protein uS5

Chain AE: 96%



- Molecule 6: 30S ribosomal protein bS6

Chain AF:  98% .



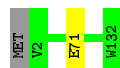
- Molecule 7: 30S ribosomal protein uS7

Chain AG:  96% ..



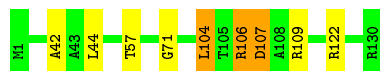
- Molecule 8: 30S ribosomal protein uS8

Chain AH:  98% ..



- Molecule 9: 30S ribosomal protein uS9

Chain AI:  93% 5% .




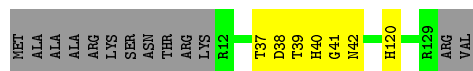
- Molecule 10: 30S ribosomal protein uS10

Chain AJ:  96% .



- Molecule 11: 30S ribosomal protein uS11

Chain AK:  85% 5% 10%



- Molecule 12: 30S ribosomal protein uS12

Chain AL:  93% 7% .



- Molecule 13: 30S ribosomal protein uS13

Chain AM:  89% 7% ..



- Molecule 14: 30S ribosomal protein uS14

Chain AN: 90% 7% ..



- Molecule 15: 30S ribosomal protein uS15

Chain AO: 97% ..



- Molecule 16: 30S ribosomal protein bS16

Chain AP: 97% ..



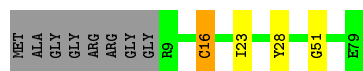
- Molecule 17: 30S ribosomal protein uS17

Chain AQ: 97% ..



- Molecule 18: 30S ribosomal protein bS18

Chain AR: 85% 10% ..



- Molecule 19: 30S ribosomal protein uS19

Chain AS: 87% 9% ..

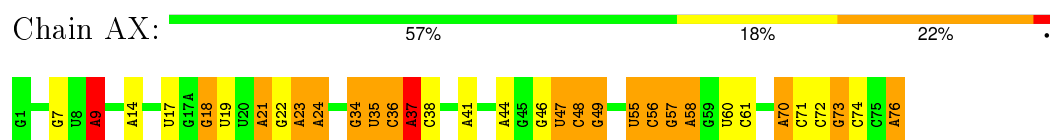


- Molecule 20: 30S ribosomal protein bS20

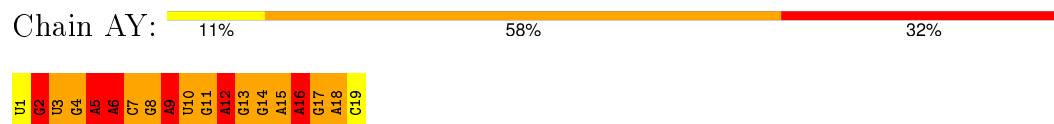
Chain AT: 92% 6% ..



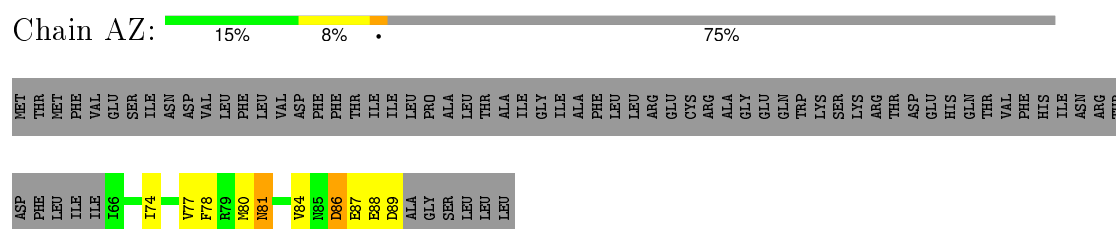
- Molecule 21: tRNA-Asp



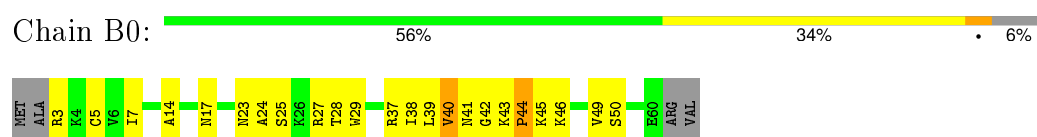
- Molecule 22: mRNA



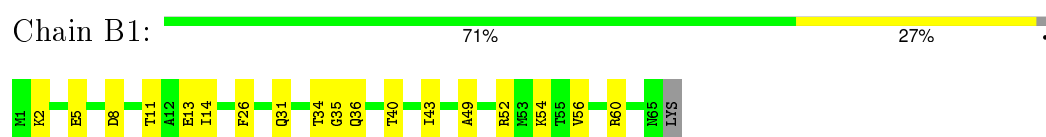
- Molecule 23: MifM



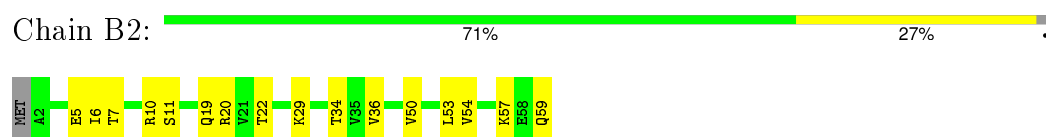
- Molecule 24: 50S ribosomal protein bL28



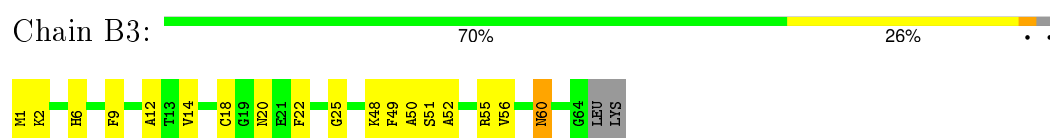
- Molecule 25: 50S ribosomal protein uL29



- Molecule 26: 50S ribosomal protein uL30

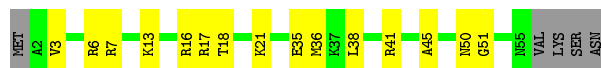


- Molecule 27: 50S ribosomal protein bL31



- Molecule 28: 50S ribosomal protein bL32

Chain B4: 




- Molecule 29: 50S ribosomal protein bL33

Chain B5: 



- Molecule 30: 50S ribosomal protein bL34

Chain B6: 



- Molecule 31: 50S ribosomal protein bL35

Chain B7: 



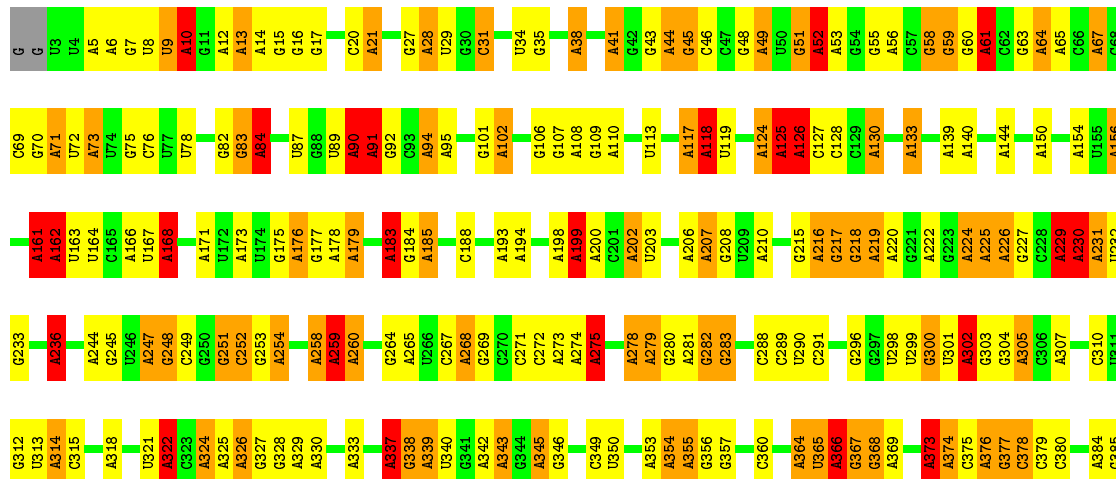
- Molecule 32: 50S ribosomal protein bL36

Chain B8: 



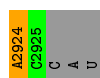
- Molecule 33: 23S ribosomal RNA

Chain BA: 



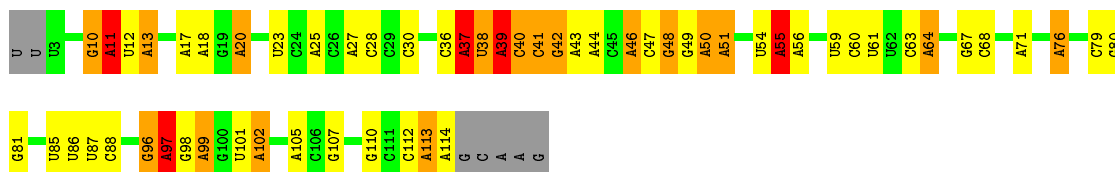
A1555	C1474	G1309	G1284	G1145	A1078	A1005	C930	C959	C785	A702	C480	C387
A1556	A1392	A1312	A1235	A1148	U1079	A1006	C931	U960	A786	G703	U481	A388
C1558	G1394	A1313	G1236	A1149	A1084	A1008	C932	C961	C787	U704	U485	A389
G1561	G1395	A1314	U1242	C1150	U1087	U1013	U934	G865	C789	A705	A486	A390
A1562	C1396	G1315	A1243	U1151	G1088	A1014	C936	A867	C791	G709	G489	A391
G1563	G1397	A1316	A1244	G1152	G1089	G1015	C937	A868	G792	G710	A490	C392
U1483	A1398	G1317	G1245	G1153	A1092	U1016	C938	U869	U793	U711	G495	U393
U1484	G1399	G1318	G1246	G1154	A1093	C1017	C939	U870	U794	C712	U496	U394
A1485	G1403	G1319	C1247	A1157	G1094	G1018	G940	A871	U795	U713	A494	U405
A1486	C1248	U1249	G1248	G1158	A1095	A1019	U942	C572	A796	A715	A495	U406
A1490	A1405	G1322	U1249	A1159	G1096	A1020	U943	G873	U797	A716	A496	A407
A1491	A1406	A1323	U1250	A1160	A1097	A1021	C944	U874	U798	C718	U497	U408
C1573	G1407	G1324	U1251	A1161	A1098	G1022	C945	U875	A799	C719	G498	G411
A1574	G1408	A1325	G1252	A1172	A1100	G1023	C946	U876	G800	C720	A500	A412
G1496	U1411	A1326	A1254	A1173	A1173	G1024	A947	G877	U799	A721	A501	A418
G1497	U1412	U1327	G1255	A1174	G1101	A1025	U948	C578	U800	A722	C502	A419
U1498	A1412	A1335	C1256	U1176	A1103	A1026	A952	G878	G804	A723	C503	U420
A1499	A1417	A1339	C1257	G1177	U1104	A1027	U953	G879	G805	A724	A504	A421
U1500	U1418	A1340	A1258	U1178	G1105	C1028	C954	C880	A808	C725	A507	G426
A1501	U1419	U1341	G1259	A1179	U1106	A1029	A956	A882	A811	A726	C508	G427
A1504	A1421	U1342	A1260	C1180	U1107	G1030	A957	A888	G812	G728	C509	A428
U1505	G1422	A1343	C1261	G1181	G1108	C1031	A958	A889	G821	U729	U510	A429
A1506	A1423	C1344	G1262	G1182	G1109	A1034	C959	U892	A821	U730	G512	C430
U1507	U1424	U1345	G1263	G1183	U1111	G1035	U960	A893	G822	G731	G513	A431
U1587	C1425	A1346	G1264	U1187	U1112	A1036	A964	A894	G823	A732	G514	G432
U1588	A1426	G1348	A1265	A1188	A1113	C1037	U966	A895	G824	U733	G515	U433
A1516	G1431	U1351	G1267	A1190	G1114	G1038	U967	A896	G825	C734	U516	U434
A1517	A1432	U1352	A1268	A1191	A1115	G1039	A897	G897	U826	U735	A517	G435
G1518	U1433	C1353	A1269	A1194	A1116	A1042	A970	G977	G827	A736	A518	A436
U1589	A1434	C1354	A1277	A1197	U1117	A1046	A971	U900	A828	C737	A519	A437
U1596	U1435	G1355	A1278	C1198	A1118	A1047	U972	U901	A829	C738	A524	C442
C1597	U1436	U1356	G1285	G1200	C1121	A1054	C975	G903	G831	A740	A525	U448
U1598	G1437	G1357	A1284	G1201	C1122	A1055	U976	A904	G832	A743	A526	A449
U1522	C1438	A1358	A1285	A1202	A1123	A1056	U977	U907	G833	A752	A527	U453
A1524	U1439	A1360	A1286	A1203	A1124	A1057	A978	A908	C834	A753	C528	U456
G1525	G1440	A1361	A1287	A1204	C1125	G1058	C980	G909	U837	A754	A530	U457
G1526	U1441	G1362	G1288	G1207	G1126	U1059	C981	A910	U838	A755	A537	U458
U1528	A1442	U1363	U1289	G1208	A1127	U1060	U982	G911	C839	A756	A538	U459
G1529	U1445	C1364	G1290	G1209	U1128	U1061	U983	C912	A840	A762	A543	A460
U1530	U1365	U1365	A1291	G1210	U1129	A1062	U984	C913	A841	A763	G544	C461
G1531	C1450	G1371	G1292	U1218	A1130	C1063	G985	U915	C843	C764	U545	A462
A1613	U1451	A1293	A1293	C1219	A1131	G1064	U986	G916	A847	A769	G546	U463
A1614	A1452	A1294	A1294	G1220	A1132	U1065	C987	A917	U848	A770	A547	U464
A1615	C1374	U1295	G1296	A1221	G1133	U1066	U988	C917	U849	A771	A548	A469
A1616	A1453	G1375	U1296	A1222	A1134	A1067	U989	A921	A850	A772	A549	A470
A1617	C1454	A1376	C1297	A1223	G1135	A1068	A991	G922	U851	A773	G550	U474
A1618	U1455	G1376	G1298	G1224	U1136	U1069	A992	A993	A852	A774	G551	A475
A1619	A1456	G1377	G1299	U1225	G1137	G1070	U992	A994	A853	A775	G552	A476
A1620	U1459	U1378	G1300	U1226	G1138	G1071	U993	A995	A854	A776	A553	U477
G1538	A1460	U1379	A1302	G1227	U1140	A1072	C997	U923	U855	C777	U554	A478
U1626	A1540	U1380	U1303	U1228	A1141	A1073	U998	A925	G856	A781	C555	U479
A1627	A1541	A1461	G1304	U1229	U1142	A1074	U999	A1003	G857	A782	G701	U480
G1628	U1542	G1382	A1305	A1230	A1143	A1075	A1003	G928	U858	U783	G702	U481
C1629	U1543	U1383	G1306	G1231	U1144	A1076	U1004	G929	U859	U784	G703	U482
U1630	A1544	C1384	U1307	G1232	U1145	A1077	U1005	G930	U860	U785	G704	U483
A1553	U1554	A1388	A1308	A1233	A1144	A1078	U1006	G931	U861	U786	G705	U484





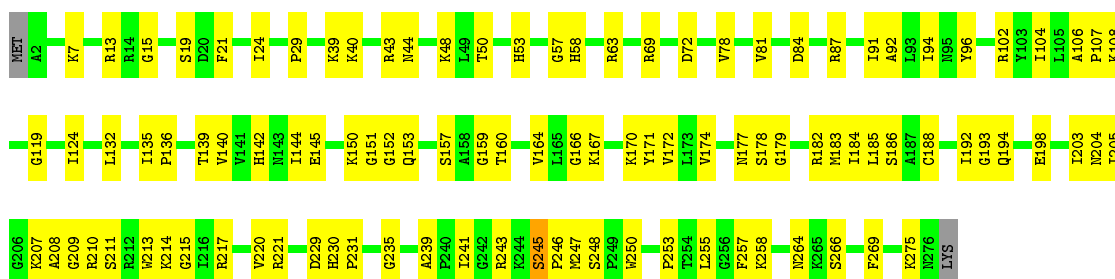
- Molecule 34: 5S ribosomal RNA

Chain BB:



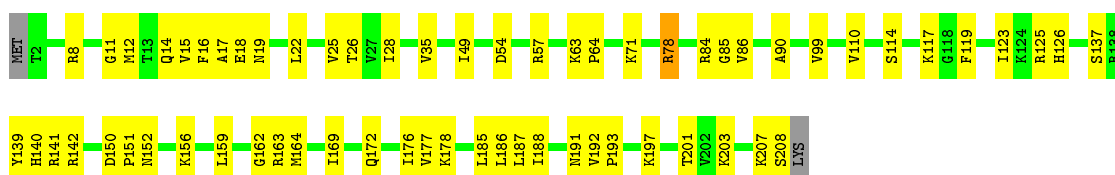
- Molecule 35: 50S ribosomal protein uL2

Chain BD:



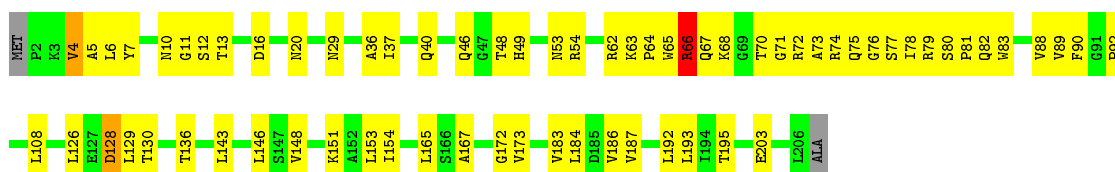
- Molecule 36: 50S ribosomal protein uL3

Chain BE:



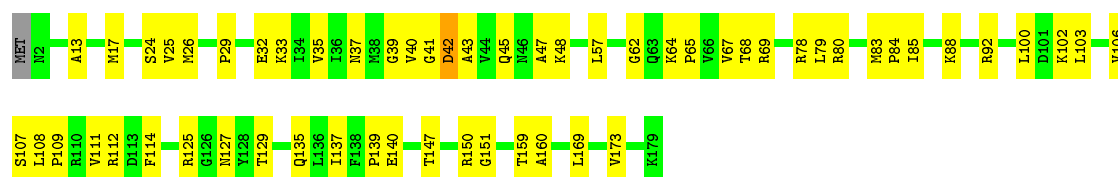
- Molecule 37: 50S ribosomal protein uL4

Chain BF:



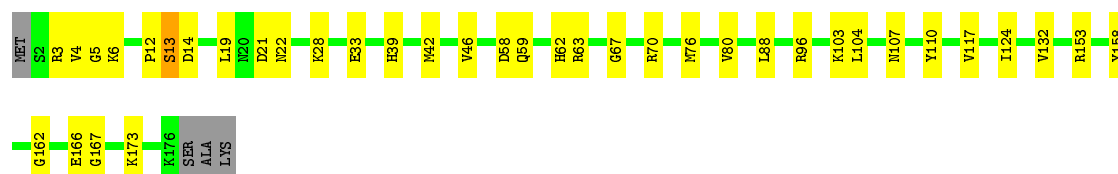
- Molecule 38: 50S ribosomal protein uL5

Chain BG:



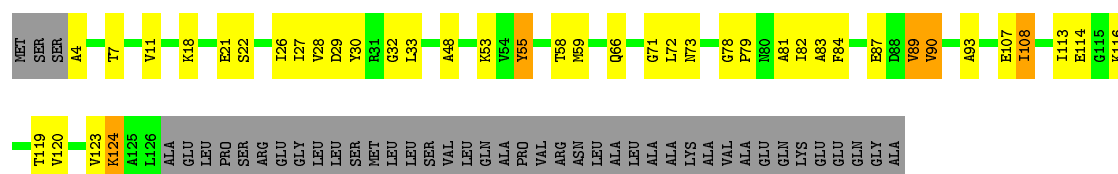
- Molecule 39: 50S ribosomal protein uL6

Chain BH: 77% 21% ..



- Molecule 40: 50S ribosomal protein uL10

Chain BJ: 49% 22% • 26%



- Molecule 41: 50S ribosomal protein uL11

Chain BK: 77% 16% • 6%



- Molecule 42: 50S ribosomal protein uL13

Chain BM: 70% 28% •



- Molecule 43: 50S ribosomal protein uL14

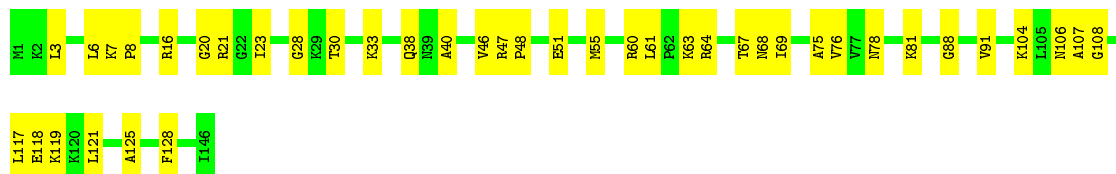
Chain BN: 72% 28%





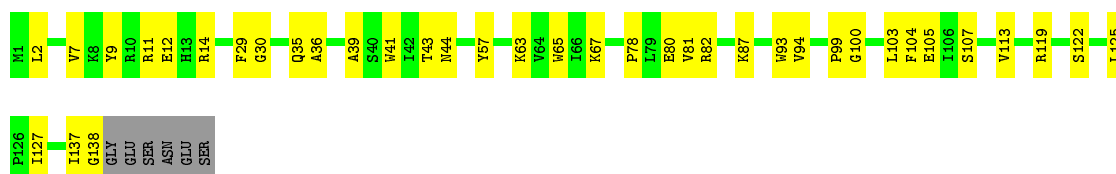
- Molecule 44: 50S ribosomal protein uL15

Chain BO: 72% 28%



- Molecule 45: 50S ribosomal protein uL16

Chain BP: 69% 26%



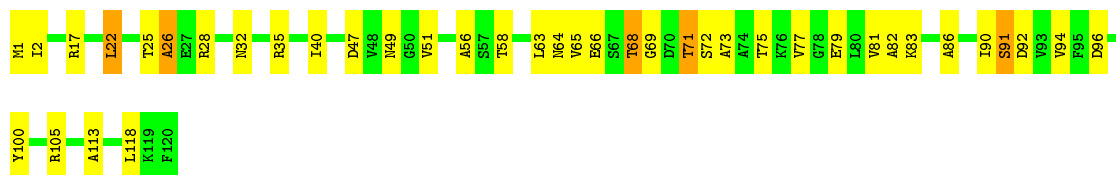
- Molecule 46: 50S ribosomal protein bL17

Chain BQ: 73% 25%



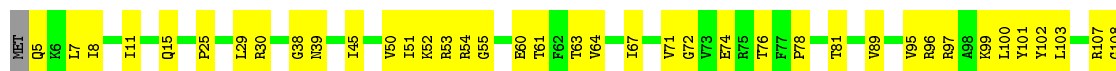
- Molecule 47: 50S ribosomal protein uL18

Chain BR: 67% 29%

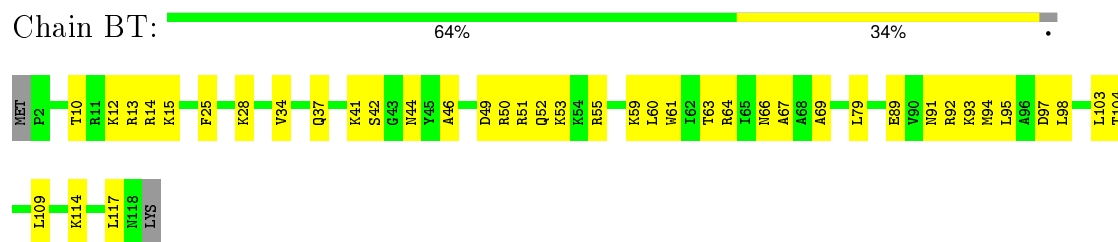


- Molecule 48: 50S ribosomal protein bL19

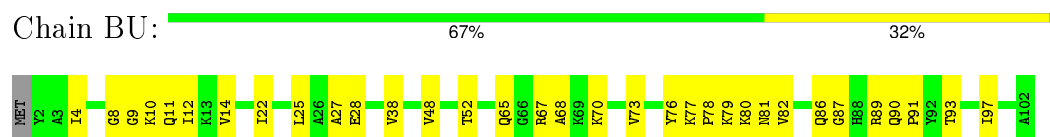
Chain BS: 65% 34%



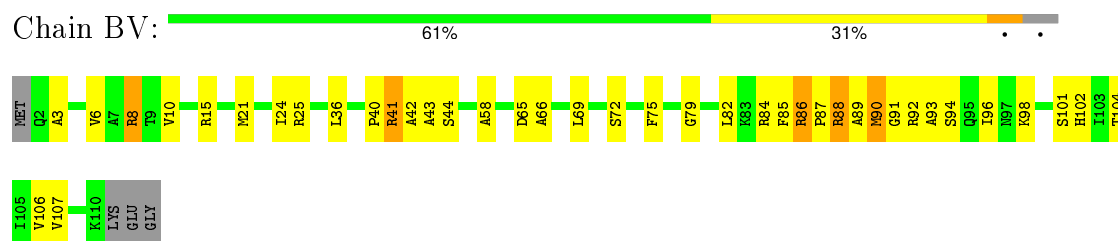
- Molecule 49: 50S ribosomal protein bL20



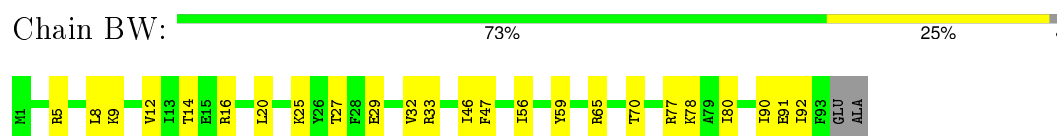
- Molecule 50: 50S ribosomal protein bL21



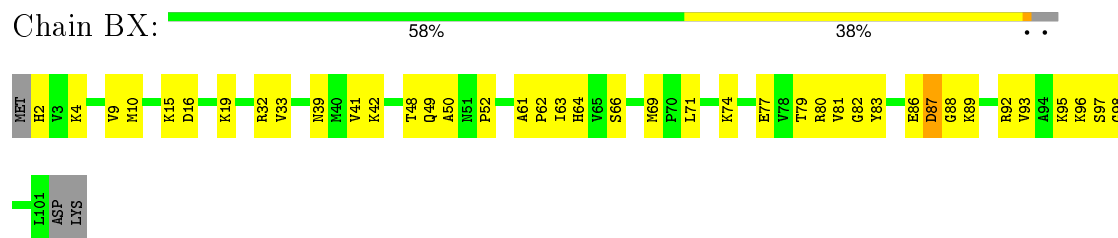
- Molecule 51: 50S ribosomal protein uL22



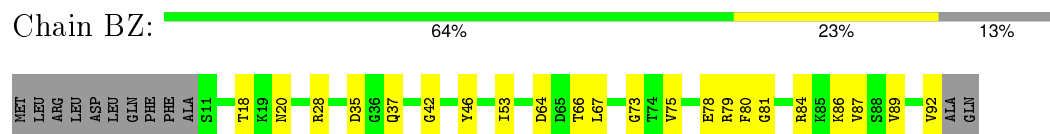
- Molecule 52: 50S ribosomal protein uL23



- Molecule 53: 50S ribosomal protein uL24



- Molecule 54: 50S ribosomal protein bL27



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	305045	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	125085	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 >2	RMSZ	# Z >2
1	AA	1.36	984/37074 (2.7%)	2.90	3806/57834 (6.6%)
10	AJ	0.28	0/408	0.39	0/507
11	AK	0.22	0/471	0.42	0/587
12	AL	0.24	0/548	0.50	0/682
13	AM	0.30	0/475	0.52	0/592
14	AN	0.21	0/240	0.48	0/297
15	AO	0.27	0/352	0.41	0/437
16	AP	0.27	0/356	0.41	0/442
17	AQ	0.27	0/344	0.44	0/427
18	AR	0.31	0/284	0.43	0/352
19	AS	0.33	0/335	0.46	0/417
2	AB	0.31	0/895	0.40	0/1117
20	AT	0.26	0/344	0.40	0/427
21	AX	1.03	30/1834 (1.6%)	2.18	104/2858 (3.6%)
22	AY	0.38	0/466	0.93	2/726 (0.3%)
23	AZ	0.50	0/106	1.02	0/122
24	B0	0.30	0/448	0.58	0/596
25	B1	0.24	0/531	0.47	0/707
26	B2	0.24	0/457	0.44	0/613
27	B3	0.27	0/513	0.43	0/683
28	B4	0.23	0/433	0.48	0/574
29	B5	0.25	0/406	0.44	0/540
3	AC	0.29	0/839	0.38	0/1047
30	B6	0.20	0/370	0.44	0/483
31	B7	0.23	0/519	0.48	0/680
32	B8	0.19	0/291	0.36	0/383
33	BA	1.40	1948/70307 (2.8%)	2.98	7636/109687 (7.0%)
34	BB	1.30	66/2678 (2.5%)	2.78	248/4174 (5.9%)
35	BD	0.27	0/2148	0.48	0/2881
36	BE	0.27	0/1597	0.47	0/2140
37	BF	0.26	0/1580	0.50	0/2132
38	BG	0.29	0/1423	0.50	0/1910
39	BH	0.23	0/1360	0.43	0/1832
4	AD	0.25	0/796	0.41	0/992

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	BJ	0.26	0/963	0.49	0/1298
41	BK	0.26	0/995	0.48	0/1346
42	BM	0.25	0/1146	0.49	0/1542
43	BN	0.28	0/927	0.47	0/1245
44	BO	0.23	0/1093	0.44	0/1457
45	BP	0.20	0/1120	0.38	0/1496
46	BQ	0.26	0/960	0.50	0/1284
47	BR	0.30	0/921	0.54	1/1236 (0.1%)
48	BS	0.24	0/949	0.44	0/1269
49	BT	0.26	0/952	0.45	0/1266
5	AE	0.26	0/660	0.46	0/822
50	BU	0.28	0/797	0.53	0/1070
51	BV	0.34	0/851	0.59	0/1146
52	BW	0.29	0/759	0.47	0/1011
53	BX	0.26	0/764	0.52	0/1022
54	BZ	0.30	0/638	0.49	0/847
6	AF	0.31	0/380	0.41	0/472
7	AG	0.26	0/612	0.39	0/762
8	AH	0.24	0/524	0.43	0/652
9	AI	0.26	0/520	0.51	0/647
All	All	1.20	3028/147759 (2.0%)	2.62	11797/221768 (5.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	36
21	AX	0	2
22	AY	0	7
33	BA	0	84
34	BB	0	2
37	BF	0	1
51	BV	0	2
All	All	0	134

All (3028) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	508	A	C8-N7	8.50	1.37	1.31
1	AA	439	A	C8-N7	8.28	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1188	A	C8-N7	8.21	1.37	1.31
1	AA	1372	A	C8-N7	8.18	1.37	1.31
33	BA	526	A	C8-N7	8.14	1.37	1.31
33	BA	2916	A	C8-N7	8.07	1.37	1.31
1	AA	631	A	C8-N7	8.05	1.37	1.31
33	BA	1417	A	C8-N7	8.02	1.37	1.31
33	BA	732	A	C8-N7	8.01	1.37	1.31
33	BA	1919	A	C8-N7	8.01	1.37	1.31
1	AA	150	A	C8-N7	8.00	1.37	1.31
1	AA	151	A	C8-N7	7.99	1.37	1.31
33	BA	2898	A	C8-N7	7.99	1.37	1.31
33	BA	374	A	C8-N7	7.98	1.37	1.31
33	BA	2793	A	C8-N7	7.98	1.37	1.31
33	BA	1814	A	C8-N7	7.98	1.37	1.31
33	BA	494	A	C8-N7	7.94	1.37	1.31
1	AA	674	A	C8-N7	7.92	1.37	1.31
33	BA	1067	A	C8-N7	7.90	1.37	1.31
33	BA	1555	A	C8-N7	7.90	1.37	1.31
33	BA	501	A	C8-N7	7.90	1.37	1.31
1	AA	899	A	C8-N7	7.90	1.37	1.31
1	AA	1133	A	C8-N7	7.90	1.37	1.31
33	BA	723	A	C8-N7	7.90	1.37	1.31
33	BA	504	A	C8-N7	7.89	1.37	1.31
33	BA	1305	A	C8-N7	7.88	1.37	1.31
33	BA	207	A	C8-N7	7.88	1.37	1.31
33	BA	2241	A	C8-N7	7.88	1.37	1.31
33	BA	1473	A	C8-N7	7.87	1.37	1.31
33	BA	2062	A	C8-N7	7.87	1.37	1.31
1	AA	457	A	C8-N7	7.86	1.37	1.31
1	AA	1358	A	C8-N7	7.86	1.37	1.31
33	BA	2254	A	C8-N7	7.86	1.37	1.31
1	AA	862	A	C8-N7	7.86	1.37	1.31
33	BA	1347	A	C8-N7	7.86	1.37	1.31
1	AA	266	A	C8-N7	7.85	1.37	1.31
1	AA	1355	A	C8-N7	7.85	1.37	1.31
33	BA	2295	A	C8-N7	7.85	1.37	1.31
33	BA	118	A	C8-N7	7.85	1.37	1.31
33	BA	2807	A	C8-N7	7.84	1.37	1.31
33	BA	448	A	C8-N7	7.84	1.37	1.31
1	AA	775	A	C8-N7	7.83	1.37	1.31
1	AA	925	A	C8-N7	7.83	1.37	1.31
33	BA	1844	A	C8-N7	7.82	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1247	A	C8-N7	7.82	1.37	1.31
1	AA	713	A	C8-N7	7.82	1.37	1.31
33	BA	1774	A	C8-N7	7.82	1.37	1.31
33	BA	1914	A	C8-N7	7.81	1.37	1.31
33	BA	2089	A	C8-N7	7.81	1.37	1.31
33	BA	224	A	C8-N7	7.81	1.37	1.31
33	BA	1434	A	C8-N7	7.80	1.37	1.31
33	BA	575	A	C8-N7	7.80	1.37	1.31
33	BA	1905	A	C8-N7	7.80	1.37	1.31
1	AA	452	A	C8-N7	7.80	1.37	1.31
1	AA	1434	A	C8-N7	7.79	1.37	1.31
1	AA	254	A	C8-N7	7.79	1.37	1.31
33	BA	647	A	C8-N7	7.79	1.37	1.31
33	BA	2908	A	C8-N7	7.79	1.36	1.31
33	BA	1302	A	C8-N7	7.78	1.36	1.31
33	BA	1078	A	C8-N7	7.78	1.36	1.31
33	BA	1201	A	C8-N7	7.78	1.36	1.31
33	BA	1784	A	C8-N7	7.78	1.36	1.31
33	BA	2134	A	C8-N7	7.78	1.36	1.31
33	BA	2375	A	C8-N7	7.78	1.36	1.31
1	AA	419	A	C8-N7	7.77	1.36	1.31
33	BA	847	A	C8-N7	7.77	1.36	1.31
33	BA	210	A	C8-N7	7.76	1.36	1.31
33	BA	1340	A	C8-N7	7.76	1.36	1.31
33	BA	2618	A	C8-N7	7.76	1.36	1.31
1	AA	837	A	C8-N7	7.76	1.36	1.31
33	BA	1579	A	C8-N7	7.75	1.36	1.31
33	BA	2083	A	C8-N7	7.75	1.36	1.31
33	BA	811	A	C8-N7	7.75	1.36	1.31
33	BA	2819	A	C8-N7	7.75	1.36	1.31
1	AA	556	A	C8-N7	7.75	1.36	1.31
1	AA	1213	A	C8-N7	7.75	1.36	1.31
33	BA	999	A	C8-N7	7.74	1.36	1.31
1	AA	1443	A	C8-N7	7.74	1.36	1.31
33	BA	183	A	C8-N7	7.74	1.36	1.31
1	AA	240	A	C8-N7	7.74	1.36	1.31
33	BA	1003	A	C8-N7	7.74	1.36	1.31
33	BA	1157	A	C8-N7	7.74	1.36	1.31
1	AA	870	A	C8-N7	7.73	1.36	1.31
33	BA	354	A	C8-N7	7.73	1.36	1.31
33	BA	2479	A	C8-N7	7.73	1.36	1.31
1	AA	189	A	C8-N7	7.73	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	208	A	C8-N7	7.73	1.36	1.31
1	AA	1466	A	C8-N7	7.72	1.36	1.31
1	AA	1257	A	C8-N7	7.72	1.36	1.31
1	AA	190	A	C8-N7	7.72	1.36	1.31
33	BA	702	A	C8-N7	7.72	1.36	1.31
33	BA	1412	A	C8-N7	7.72	1.36	1.31
33	BA	1941	A	C8-N7	7.72	1.36	1.31
33	BA	314	A	C8-N7	7.72	1.36	1.31
1	AA	139	A	C8-N7	7.71	1.36	1.31
21	AX	23	A	C8-N7	7.71	1.36	1.31
33	BA	1020	A	C8-N7	7.71	1.36	1.31
33	BA	1339	A	C8-N7	7.71	1.36	1.31
33	BA	2362	A	C8-N7	7.71	1.36	1.31
1	AA	491	A	C8-N7	7.71	1.36	1.31
33	BA	1119	A	C8-N7	7.71	1.36	1.31
1	AA	738	A	C8-N7	7.70	1.36	1.31
33	BA	2042	A	C8-N7	7.70	1.36	1.31
33	BA	2187	A	C8-N7	7.70	1.36	1.31
1	AA	28	A	C8-N7	7.70	1.36	1.31
33	BA	1961	A	C8-N7	7.70	1.36	1.31
33	BA	2480	A	C8-N7	7.70	1.36	1.31
1	AA	1333	A	C8-N7	7.69	1.36	1.31
1	AA	1541	A	C8-N7	7.69	1.36	1.31
33	BA	2398	A	C8-N7	7.69	1.36	1.31
1	AA	1503	A	C8-N7	7.69	1.36	1.31
33	BA	2152	A	C8-N7	7.69	1.36	1.31
1	AA	737	A	C8-N7	7.69	1.36	1.31
1	AA	228	A	C8-N7	7.69	1.36	1.31
1	AA	422	A	C8-N7	7.69	1.36	1.31
1	AA	924	A	C8-N7	7.69	1.36	1.31
1	AA	1056	A	C8-N7	7.69	1.36	1.31
33	BA	173	A	C8-N7	7.69	1.36	1.31
33	BA	1123	A	C8-N7	7.69	1.36	1.31
1	AA	988	A	C8-N7	7.69	1.36	1.31
1	AA	1050	A	C8-N7	7.69	1.36	1.31
1	AA	206	A	C8-N7	7.68	1.36	1.31
1	AA	923	A	C8-N7	7.68	1.36	1.31
33	BA	199	A	C8-N7	7.68	1.36	1.31
33	BA	273	A	C8-N7	7.68	1.36	1.31
33	BA	740	A	C8-N7	7.68	1.36	1.31
33	BA	1516	A	C8-N7	7.68	1.36	1.31
1	AA	367	A	C8-N7	7.68	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	781	A	C8-N7	7.68	1.36	1.31
33	BA	1381	A	C8-N7	7.68	1.36	1.31
33	BA	2330	A	C8-N7	7.68	1.36	1.31
1	AA	118	A	C8-N7	7.68	1.36	1.31
1	AA	170	A	C8-N7	7.68	1.36	1.31
1	AA	928	A	C8-N7	7.68	1.36	1.31
33	BA	2670	A	C8-N7	7.68	1.36	1.31
1	AA	117	A	C8-N7	7.68	1.36	1.31
1	AA	232	A	C8-N7	7.68	1.36	1.31
33	BA	1084	A	C8-N7	7.68	1.36	1.31
33	BA	2220	A	C8-N7	7.68	1.36	1.31
1	AA	500	A	C8-N7	7.68	1.36	1.31
33	BA	124	A	C8-N7	7.68	1.36	1.31
1	AA	506	A	C8-N7	7.68	1.36	1.31
1	AA	777	A	C8-N7	7.68	1.36	1.31
33	BA	166	A	C8-N7	7.68	1.36	1.31
33	BA	333	A	C8-N7	7.68	1.36	1.31
34	BB	102	A	C8-N7	7.68	1.36	1.31
1	AA	507	A	C8-N7	7.67	1.36	1.31
1	AA	658	A	C8-N7	7.67	1.36	1.31
1	AA	1254	A	C8-N7	7.67	1.36	1.31
33	BA	274	A	C8-N7	7.67	1.36	1.31
33	BA	637	A	C8-N7	7.67	1.36	1.31
33	BA	1636	A	C8-N7	7.67	1.36	1.31
1	AA	386	A	C8-N7	7.67	1.36	1.31
33	BA	1046	A	C8-N7	7.67	1.36	1.31
33	BA	1113	A	C8-N7	7.67	1.36	1.31
33	BA	2767	A	C8-N7	7.67	1.36	1.31
33	BA	2875	A	C8-N7	7.67	1.36	1.31
33	BA	389	A	C8-N7	7.67	1.36	1.31
33	BA	1314	A	C8-N7	7.67	1.36	1.31
1	AA	171	A	C8-N7	7.67	1.36	1.31
33	BA	219	A	C8-N7	7.67	1.36	1.31
33	BA	1161	A	C8-N7	7.67	1.36	1.31
1	AA	1006	A	C8-N7	7.67	1.36	1.31
33	BA	1034	A	C8-N7	7.67	1.36	1.31
33	BA	1202	A	C8-N7	7.67	1.36	1.31
1	AA	438	A	C8-N7	7.67	1.36	1.31
33	BA	322	A	C8-N7	7.67	1.36	1.31
33	BA	957	A	C8-N7	7.67	1.36	1.31
33	BA	64	A	C8-N7	7.66	1.36	1.31
33	BA	543	A	C8-N7	7.66	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1532	A	C8-N7	7.66	1.36	1.31
33	BA	1906	A	C8-N7	7.66	1.36	1.31
33	BA	421	A	C8-N7	7.66	1.36	1.31
33	BA	1061	A	C8-N7	7.66	1.36	1.31
34	BB	55	A	C8-N7	7.66	1.36	1.31
1	AA	202	A	C8-N7	7.66	1.36	1.31
33	BA	179	A	C8-N7	7.66	1.36	1.31
33	BA	965	A	C8-N7	7.66	1.36	1.31
33	BA	1406	A	C8-N7	7.66	1.36	1.31
1	AA	211	A	C8-N7	7.66	1.36	1.31
33	BA	991	A	C8-N7	7.66	1.36	1.31
33	BA	44	A	C8-N7	7.66	1.36	1.31
33	BA	161	A	C8-N7	7.66	1.36	1.31
33	BA	244	A	C8-N7	7.66	1.36	1.31
33	BA	1144	A	C8-N7	7.66	1.36	1.31
33	BA	91	A	C8-N7	7.65	1.36	1.31
33	BA	229	A	C8-N7	7.65	1.36	1.31
1	AA	1512	A	C8-N7	7.65	1.36	1.31
33	BA	618	A	C8-N7	7.65	1.36	1.31
33	BA	1325	A	C8-N7	7.65	1.36	1.31
33	BA	1601	A	C8-N7	7.65	1.36	1.31
33	BA	2141	A	C8-N7	7.65	1.36	1.31
1	AA	721	A	C8-N7	7.65	1.36	1.31
1	AA	1470	A	C8-N7	7.65	1.36	1.31
33	BA	1746	A	C8-N7	7.65	1.36	1.31
33	BA	1788	A	C8-N7	7.65	1.36	1.31
33	BA	1966	A	C8-N7	7.65	1.36	1.31
1	AA	62	A	C8-N7	7.65	1.36	1.31
1	AA	1419	A	C8-N7	7.65	1.36	1.31
33	BA	1115	A	C8-N7	7.65	1.36	1.31
1	AA	1342	A	C8-N7	7.65	1.36	1.31
33	BA	28	A	C8-N7	7.65	1.36	1.31
33	BA	2601	A	C8-N7	7.65	1.36	1.31
33	BA	758	A	C8-N7	7.65	1.36	1.31
33	BA	1713	A	C8-N7	7.65	1.36	1.31
33	BA	1722	A	C8-N7	7.65	1.36	1.31
33	BA	329	A	C8-N7	7.64	1.36	1.31
33	BA	821	A	C8-N7	7.64	1.36	1.31
1	AA	296	A	C8-N7	7.64	1.36	1.31
1	AA	501	A	C8-N7	7.64	1.36	1.31
1	AA	323	A	C8-N7	7.64	1.36	1.31
1	AA	1140	A	C8-N7	7.64	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	342	A	C8-N7	7.64	1.36	1.31
33	BA	1504	A	C8-N7	7.64	1.36	1.31
33	BA	1815	A	C8-N7	7.64	1.36	1.31
1	AA	178	A	C8-N7	7.64	1.36	1.31
1	AA	203	A	C8-N7	7.64	1.36	1.31
1	AA	258	A	C8-N7	7.64	1.36	1.31
1	AA	651	A	C8-N7	7.64	1.36	1.31
1	AA	690	A	C8-N7	7.64	1.36	1.31
33	BA	125	A	C8-N7	7.64	1.36	1.31
33	BA	281	A	C8-N7	7.64	1.36	1.31
34	BB	18	A	C8-N7	7.64	1.36	1.31
1	AA	1488	A	C8-N7	7.64	1.36	1.31
33	BA	2778	A	C8-N7	7.64	1.36	1.31
1	AA	671	A	C8-N7	7.64	1.36	1.31
1	AA	1178	A	C8-N7	7.64	1.36	1.31
33	BA	1269	A	C8-N7	7.64	1.36	1.31
1	AA	401	A	C8-N7	7.63	1.36	1.31
1	AA	968	A	C8-N7	7.63	1.36	1.31
33	BA	67	A	C8-N7	7.63	1.36	1.31
33	BA	1142	A	C8-N7	7.63	1.36	1.31
33	BA	1654	A	C8-N7	7.63	1.36	1.31
33	BA	1797	A	C8-N7	7.63	1.36	1.31
33	BA	1930	A	C8-N7	7.63	1.36	1.31
33	BA	2526	A	C8-N7	7.63	1.36	1.31
1	AA	31	A	C8-N7	7.63	1.36	1.31
1	AA	159	A	C8-N7	7.63	1.36	1.31
1	AA	371	A	C8-N7	7.63	1.36	1.31
33	BA	144	A	C8-N7	7.63	1.36	1.31
33	BA	202	A	C8-N7	7.63	1.36	1.31
33	BA	652	A	C8-N7	7.63	1.36	1.31
33	BA	1116	A	C8-N7	7.63	1.36	1.31
33	BA	1287	A	C8-N7	7.63	1.36	1.31
33	BA	2673	A	C8-N7	7.63	1.36	1.31
34	BB	71	A	C8-N7	7.63	1.36	1.31
1	AA	1422	A	C8-N7	7.63	1.36	1.31
33	BA	1130	A	C8-N7	7.63	1.36	1.31
1	AA	1092	A	C8-N7	7.63	1.36	1.31
1	AA	1185	A	C8-N7	7.63	1.36	1.31
1	AA	1210	A	C8-N7	7.63	1.36	1.31
1	AA	1502	A	C8-N7	7.63	1.36	1.31
21	AX	58	A	C8-N7	7.63	1.36	1.31
33	BA	94	A	C8-N7	7.63	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	154	A	C8-N7	7.63	1.36	1.31
33	BA	1230	A	C8-N7	7.63	1.36	1.31
33	BA	2071	A	C8-N7	7.63	1.36	1.31
33	BA	2683	A	C8-N7	7.63	1.36	1.31
1	AA	1077	A	C8-N7	7.63	1.36	1.31
33	BA	476	A	C8-N7	7.63	1.36	1.31
33	BA	717	A	C8-N7	7.63	1.36	1.31
33	BA	2087	A	C8-N7	7.63	1.36	1.31
33	BA	2032	A	C8-N7	7.62	1.36	1.31
33	BA	2447	A	C8-N7	7.62	1.36	1.31
33	BA	952	A	C8-N7	7.62	1.36	1.31
33	BA	1677	A	C8-N7	7.62	1.36	1.31
33	BA	1948	A	C8-N7	7.62	1.36	1.31
33	BA	2505	A	C8-N7	7.62	1.36	1.31
33	BA	2593	A	C8-N7	7.62	1.36	1.31
33	BA	206	A	C8-N7	7.62	1.36	1.31
33	BA	345	A	C8-N7	7.62	1.36	1.31
33	BA	1189	A	C8-N7	7.62	1.36	1.31
1	AA	801	A	C8-N7	7.62	1.36	1.31
1	AA	53	A	C8-N7	7.62	1.36	1.31
1	AA	148	A	C8-N7	7.62	1.36	1.31
1	AA	1479	A	C8-N7	7.62	1.36	1.31
33	BA	1308	A	C8-N7	7.62	1.36	1.31
33	BA	1534	A	C8-N7	7.62	1.36	1.31
33	BA	2165	A	C8-N7	7.62	1.36	1.31
33	BA	2590	A	C8-N7	7.62	1.36	1.31
33	BA	2912	A	C8-N7	7.62	1.36	1.31
1	AA	1455	A	C8-N7	7.62	1.36	1.31
33	BA	278	A	C8-N7	7.62	1.36	1.31
33	BA	2088	A	C8-N7	7.62	1.36	1.31
34	BB	17	A	C8-N7	7.62	1.36	1.31
1	AA	725	A	C8-N7	7.62	1.36	1.31
1	AA	1437	A	C8-N7	7.62	1.36	1.31
33	BA	1925	A	C8-N7	7.62	1.36	1.31
1	AA	129	A	C8-N7	7.61	1.36	1.31
1	AA	542	A	C8-N7	7.61	1.36	1.31
1	AA	664	A	C8-N7	7.61	1.36	1.31
1	AA	703	A	C8-N7	7.61	1.36	1.31
33	BA	5	A	C8-N7	7.61	1.36	1.31
33	BA	216	A	C8-N7	7.61	1.36	1.31
33	BA	373	A	C8-N7	7.61	1.36	1.31
33	BA	2034	A	C8-N7	7.61	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2686	A	C8-N7	7.61	1.36	1.31
1	AA	10	A	C8-N7	7.61	1.36	1.31
1	AA	1022	A	C8-N7	7.61	1.36	1.31
1	AA	1320	A	C8-N7	7.61	1.36	1.31
33	BA	2307	A	C8-N7	7.61	1.36	1.31
1	AA	669	A	C8-N7	7.61	1.36	1.31
1	AA	757	A	C8-N7	7.61	1.36	1.31
1	AA	771	A	C8-N7	7.61	1.36	1.31
1	AA	1115	A	C8-N7	7.61	1.36	1.31
1	AA	1225	A	C8-N7	7.61	1.36	1.31
33	BA	418	A	C8-N7	7.61	1.36	1.31
33	BA	867	A	C8-N7	7.61	1.36	1.31
33	BA	1055	A	C8-N7	7.61	1.36	1.31
1	AA	389	A	C8-N7	7.61	1.36	1.31
1	AA	541	A	C8-N7	7.61	1.36	1.31
33	BA	388	A	C8-N7	7.61	1.36	1.31
33	BA	1593	A	C8-N7	7.61	1.36	1.31
1	AA	251	A	C8-N7	7.61	1.36	1.31
1	AA	282	A	C8-N7	7.61	1.36	1.31
1	AA	569	A	C8-N7	7.61	1.36	1.31
1	AA	985	A	C8-N7	7.61	1.36	1.31
1	AA	1090	A	C8-N7	7.61	1.36	1.31
33	BA	477	A	C8-N7	7.61	1.36	1.31
33	BA	1005	A	C8-N7	7.61	1.36	1.31
33	BA	1286	A	C8-N7	7.61	1.36	1.31
33	BA	1483	A	C8-N7	7.61	1.36	1.31
1	AA	1017	A	C8-N7	7.61	1.36	1.31
1	AA	1417	A	C8-N7	7.61	1.36	1.31
1	AA	352	A	C8-N7	7.60	1.36	1.31
1	AA	824	A	C8-N7	7.60	1.36	1.31
33	BA	888	A	C8-N7	7.60	1.36	1.31
33	BA	1995	A	C8-N7	7.60	1.36	1.31
1	AA	485	A	C8-N7	7.60	1.36	1.31
33	BA	1014	A	C8-N7	7.60	1.36	1.31
33	BA	1026	A	C8-N7	7.60	1.36	1.31
1	AA	67	A	C8-N7	7.60	1.36	1.31
1	AA	618	A	C8-N7	7.60	1.36	1.31
1	AA	910	A	C8-N7	7.60	1.36	1.31
1	AA	1298	A	C8-N7	7.60	1.36	1.31
33	BA	6	A	C8-N7	7.60	1.36	1.31
33	BA	200	A	C8-N7	7.60	1.36	1.31
33	BA	572	A	C8-N7	7.60	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1008	A	C8-N7	7.60	1.36	1.31
33	BA	1724	A	C8-N7	7.60	1.36	1.31
33	BA	2902	A	C8-N7	7.60	1.36	1.31
1	AA	357	A	C8-N7	7.60	1.36	1.31
1	AA	762	A	C8-N7	7.60	1.36	1.31
1	AA	786	A	C8-N7	7.60	1.36	1.31
1	AA	791	A	C8-N7	7.60	1.36	1.31
1	AA	1207	A	C8-N7	7.60	1.36	1.31
33	BA	646	A	C8-N7	7.60	1.36	1.31
33	BA	1947	A	C8-N7	7.60	1.36	1.31
33	BA	2461	A	C8-N7	7.60	1.36	1.31
33	BA	2500	A	C8-N7	7.60	1.36	1.31
33	BA	2893	A	C8-N7	7.60	1.36	1.31
34	BB	27	A	C8-N7	7.60	1.36	1.31
1	AA	463	A	C8-N7	7.60	1.36	1.31
1	AA	816	A	C8-N7	7.60	1.36	1.31
33	BA	49	A	C8-N7	7.60	1.36	1.31
33	BA	1876	A	C8-N7	7.60	1.36	1.31
33	BA	2357	A	C8-N7	7.60	1.36	1.31
34	BB	64	A	C8-N7	7.60	1.36	1.31
1	AA	423	A	C8-N7	7.59	1.36	1.31
1	AA	929	A	C8-N7	7.59	1.36	1.31
1	AA	1102	A	C8-N7	7.59	1.36	1.31
1	AA	1386	A	C8-N7	7.59	1.36	1.31
33	BA	547	A	C8-N7	7.59	1.36	1.31
33	BA	925	A	C8-N7	7.59	1.36	1.31
33	BA	1141	A	C8-N7	7.59	1.36	1.31
33	BA	1244	A	C8-N7	7.59	1.36	1.31
33	BA	1675	A	C8-N7	7.59	1.36	1.31
33	BA	2146	A	C8-N7	7.59	1.36	1.31
33	BA	2769	A	C8-N7	7.59	1.36	1.31
33	BA	2860	A	C8-N7	7.59	1.36	1.31
1	AA	236	A	C8-N7	7.59	1.36	1.31
33	BA	677	A	C8-N7	7.59	1.36	1.31
33	BA	2668	A	C8-N7	7.59	1.36	1.31
33	BA	2876	A	C8-N7	7.59	1.36	1.31
1	AA	404	A	C8-N7	7.59	1.36	1.31
21	AX	21	A	C8-N7	7.59	1.36	1.31
33	BA	1445	A	C8-N7	7.59	1.36	1.31
33	BA	1540	A	C8-N7	7.59	1.36	1.31
33	BA	2754	A	C8-N7	7.59	1.36	1.31
1	AA	382	A	C8-N7	7.59	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	456	A	C8-N7	7.59	1.36	1.31
1	AA	544	A	C8-N7	7.59	1.36	1.31
33	BA	1499	A	C8-N7	7.59	1.36	1.31
33	BA	2722	A	C8-N7	7.59	1.36	1.31
1	AA	504	A	C8-N7	7.59	1.36	1.31
1	AA	1128	A	C8-N7	7.59	1.36	1.31
33	BA	198	A	C8-N7	7.59	1.36	1.31
33	BA	325	A	C8-N7	7.59	1.36	1.31
33	BA	438	A	C8-N7	7.59	1.36	1.31
33	BA	592	A	C8-N7	7.59	1.36	1.31
33	BA	2595	A	C8-N7	7.59	1.36	1.31
1	AA	522	A	C8-N7	7.59	1.36	1.31
1	AA	974	A	C8-N7	7.59	1.36	1.31
1	AA	1180	A	C8-N7	7.59	1.36	1.31
1	AA	1271	A	C8-N7	7.59	1.36	1.31
33	BA	102	A	C8-N7	7.59	1.36	1.31
33	BA	593	A	C8-N7	7.59	1.36	1.31
33	BA	786	A	C8-N7	7.59	1.36	1.31
33	BA	1025	A	C8-N7	7.59	1.36	1.31
33	BA	1175	A	C8-N7	7.59	1.36	1.31
1	AA	828	A	C8-N7	7.58	1.36	1.31
33	BA	1097	A	C8-N7	7.58	1.36	1.31
1	AA	18	A	C8-N7	7.58	1.36	1.31
1	AA	209	A	C8-N7	7.58	1.36	1.31
1	AA	474	A	C8-N7	7.58	1.36	1.31
1	AA	825	A	C8-N7	7.58	1.36	1.31
33	BA	470	A	C8-N7	7.58	1.36	1.31
33	BA	490	A	C8-N7	7.58	1.36	1.31
33	BA	561	A	C8-N7	7.58	1.36	1.31
33	BA	851	A	C8-N7	7.58	1.36	1.31
33	BA	896	A	C8-N7	7.58	1.36	1.31
33	BA	1313	A	C8-N7	7.58	1.36	1.31
33	BA	1592	A	C8-N7	7.58	1.36	1.31
33	BA	2030	A	C8-N7	7.58	1.36	1.31
33	BA	2317	A	C8-N7	7.58	1.36	1.31
1	AA	34	A	C8-N7	7.58	1.36	1.31
1	AA	306	A	C8-N7	7.58	1.36	1.31
1	AA	1259	A	C8-N7	7.58	1.36	1.31
1	AA	1359	A	C8-N7	7.58	1.36	1.31
33	BA	782	A	C8-N7	7.58	1.36	1.31
33	BA	1679	A	C8-N7	7.58	1.36	1.31
33	BA	1735	A	C8-N7	7.58	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2343	A	C8-N7	7.58	1.36	1.31
33	BA	247	A	C8-N7	7.58	1.36	1.31
33	BA	1432	A	C8-N7	7.58	1.36	1.31
33	BA	1697	A	C8-N7	7.58	1.36	1.31
34	BB	39	A	C8-N7	7.58	1.36	1.31
1	AA	52	A	C8-N7	7.58	1.36	1.31
1	AA	1176	A	C8-N7	7.58	1.36	1.31
33	BA	762	A	C8-N7	7.58	1.36	1.31
33	BA	2356	A	C8-N7	7.58	1.36	1.31
33	BA	2477	A	C8-N7	7.58	1.36	1.31
34	BB	25	A	C8-N7	7.58	1.36	1.31
1	AA	440	A	C8-N7	7.58	1.36	1.31
1	AA	1236	A	C8-N7	7.58	1.36	1.31
1	AA	1349	A	C8-N7	7.58	1.36	1.31
1	AA	1486	A	C8-N7	7.58	1.36	1.31
33	BA	337	A	C8-N7	7.58	1.36	1.31
33	BA	1224	A	C8-N7	7.58	1.36	1.31
33	BA	1323	A	C8-N7	7.58	1.36	1.31
33	BA	1789	A	C8-N7	7.58	1.36	1.31
33	BA	2170	A	C8-N7	7.58	1.36	1.31
33	BA	2845	A	C8-N7	7.58	1.36	1.31
1	AA	477	A	C8-N7	7.57	1.36	1.31
1	AA	568	A	C8-N7	7.57	1.36	1.31
1	AA	611	A	C8-N7	7.57	1.36	1.31
1	AA	975	A	C8-N7	7.57	1.36	1.31
1	AA	1266	A	C8-N7	7.57	1.36	1.31
1	AA	1283	A	C8-N7	7.57	1.36	1.31
33	BA	507	A	C8-N7	7.57	1.36	1.31
1	AA	581	A	C8-N7	7.57	1.36	1.31
33	BA	1388	A	C8-N7	7.57	1.36	1.31
33	BA	1424	A	C8-N7	7.57	1.36	1.31
1	AA	142	A	C8-N7	7.57	1.36	1.31
1	AA	672	A	C8-N7	7.57	1.36	1.31
1	AA	1048	A	C8-N7	7.57	1.36	1.31
1	AA	1456	A	C8-N7	7.57	1.36	1.31
33	BA	2119	A	C8-N7	7.57	1.36	1.31
33	BA	2256	A	C8-N7	7.57	1.36	1.31
33	BA	2750	A	C8-N7	7.57	1.36	1.31
33	BA	2900	A	C8-N7	7.57	1.36	1.31
33	BA	178	A	C8-N7	7.57	1.36	1.31
33	BA	2455	A	C8-N7	7.57	1.36	1.31
1	AA	278	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	314	A	C8-N7	7.57	1.36	1.31
1	AA	529	A	C8-N7	7.57	1.36	1.31
1	AA	743	A	C8-N7	7.57	1.36	1.31
1	AA	1289	A	C8-N7	7.57	1.36	1.31
1	AA	1509	A	C8-N7	7.57	1.36	1.31
33	BA	139	A	C8-N7	7.57	1.36	1.31
33	BA	369	A	C8-N7	7.57	1.36	1.31
33	BA	2276	A	C8-N7	7.57	1.36	1.31
33	BA	2629	A	C8-N7	7.57	1.36	1.31
1	AA	831	A	C8-N7	7.57	1.36	1.31
1	AA	1120	A	C8-N7	7.57	1.36	1.31
1	AA	1405	A	C8-N7	7.57	1.36	1.31
33	BA	133	A	C8-N7	7.57	1.36	1.31
33	BA	770	A	C8-N7	7.57	1.36	1.31
33	BA	1686	A	C8-N7	7.57	1.36	1.31
33	BA	1850	A	C8-N7	7.57	1.36	1.31
33	BA	2262	A	C8-N7	7.57	1.36	1.31
33	BA	2482	A	C8-N7	7.57	1.36	1.31
33	BA	2498	A	C8-N7	7.57	1.36	1.31
33	BA	2837	A	C8-N7	7.57	1.36	1.31
1	AA	582	A	C8-N7	7.56	1.36	1.31
1	AA	715	A	C8-N7	7.56	1.36	1.31
33	BA	763	A	C8-N7	7.56	1.36	1.31
33	BA	2777	A	C8-N7	7.56	1.36	1.31
34	BB	114	A	C8-N7	7.56	1.36	1.31
1	AA	415	A	C8-N7	7.56	1.36	1.31
1	AA	1407	A	C8-N7	7.56	1.36	1.31
1	AA	1435	A	C8-N7	7.56	1.36	1.31
21	AX	44	A	C8-N7	7.56	1.36	1.31
33	BA	110	A	C8-N7	7.56	1.36	1.31
33	BA	582	A	C8-N7	7.56	1.36	1.31
33	BA	917	A	C8-N7	7.56	1.36	1.31
33	BA	922	A	C8-N7	7.56	1.36	1.31
33	BA	1882	A	C8-N7	7.56	1.36	1.31
33	BA	2782	A	C8-N7	7.56	1.36	1.31
1	AA	173	A	C8-N7	7.56	1.36	1.31
1	AA	1028	A	C8-N7	7.56	1.36	1.31
1	AA	1054	A	C8-N7	7.56	1.36	1.31
33	BA	364	A	C8-N7	7.56	1.36	1.31
33	BA	479	A	C8-N7	7.56	1.36	1.31
1	AA	704	A	C8-N7	7.56	1.36	1.31
1	AA	1014	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	1205	A	C8-N7	7.56	1.36	1.31
33	BA	65	A	C8-N7	7.56	1.36	1.31
33	BA	279	A	C8-N7	7.56	1.36	1.31
33	BA	553	A	C8-N7	7.56	1.36	1.31
33	BA	727	A	C8-N7	7.56	1.36	1.31
33	BA	1210	A	C8-N7	7.56	1.36	1.31
33	BA	2000	A	C8-N7	7.56	1.36	1.31
33	BA	2078	A	C8-N7	7.56	1.36	1.31
33	BA	2542	A	C8-N7	7.56	1.36	1.31
33	BA	2826	A	C8-N7	7.56	1.36	1.31
33	BA	2854	A	C8-N7	7.56	1.36	1.31
34	BB	76	A	C8-N7	7.56	1.36	1.31
33	BA	61	A	C8-N7	7.56	1.36	1.31
33	BA	73	A	C8-N7	7.56	1.36	1.31
33	BA	222	A	C8-N7	7.56	1.36	1.31
33	BA	1179	A	C8-N7	7.56	1.36	1.31
33	BA	1456	A	C8-N7	7.56	1.36	1.31
33	BA	2383	A	C8-N7	7.56	1.36	1.31
33	BA	2606	A	C8-N7	7.56	1.36	1.31
33	BA	2700	A	C8-N7	7.56	1.36	1.31
33	BA	1812	A	C8-N7	7.56	1.36	1.31
1	AA	803	A	C8-N7	7.55	1.36	1.31
1	AA	1260	A	C8-N7	7.55	1.36	1.31
1	AA	1270	A	C8-N7	7.55	1.36	1.31
1	AA	1510	A	C8-N7	7.55	1.36	1.31
21	AX	41	A	C8-N7	7.55	1.36	1.31
33	BA	126	A	C8-N7	7.55	1.36	1.31
33	BA	1233	A	C8-N7	7.55	1.36	1.31
33	BA	1398	A	C8-N7	7.55	1.36	1.31
33	BA	1631	A	C8-N7	7.55	1.36	1.31
33	BA	1743	A	C8-N7	7.55	1.36	1.31
33	BA	2049	A	C8-N7	7.55	1.36	1.31
1	AA	1200	A	C8-N7	7.55	1.36	1.31
1	AA	1327	A	C8-N7	7.55	1.36	1.31
33	BA	302	A	C8-N7	7.55	1.36	1.31
33	BA	1361	A	C8-N7	7.55	1.36	1.31
33	BA	2389	A	C8-N7	7.55	1.36	1.31
1	AA	344	A	C8-N7	7.55	1.36	1.31
1	AA	685	A	C8-N7	7.55	1.36	1.31
1	AA	1369	A	C8-N7	7.55	1.36	1.31
21	AX	14	A	C8-N7	7.55	1.36	1.31
33	BA	162	A	C8-N7	7.55	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	699	A	C8-N7	7.55	1.36	1.31
33	BA	1029	A	C8-N7	7.55	1.36	1.31
33	BA	1734	A	C8-N7	7.55	1.36	1.31
33	BA	1885	A	C8-N7	7.55	1.36	1.31
33	BA	2507	A	C8-N7	7.55	1.36	1.31
34	BB	50	A	C8-N7	7.55	1.36	1.31
1	AA	1425	A	C8-N7	7.55	1.36	1.31
33	BA	412	A	C8-N7	7.55	1.36	1.31
33	BA	1021	A	C8-N7	7.55	1.36	1.31
33	BA	1465	A	C8-N7	7.55	1.36	1.31
33	BA	1791	A	C8-N7	7.55	1.36	1.31
33	BA	2835	A	C8-N7	7.55	1.36	1.31
33	BA	1423	A	C8-N7	7.55	1.36	1.31
1	AA	459	A	C8-N7	7.55	1.36	1.31
33	BA	318	A	C8-N7	7.55	1.36	1.31
33	BA	808	A	C8-N7	7.55	1.36	1.31
33	BA	908	A	C8-N7	7.55	1.36	1.31
33	BA	1066	A	C8-N7	7.55	1.36	1.31
33	BA	1614	A	C8-N7	7.55	1.36	1.31
33	BA	2155	A	C8-N7	7.55	1.36	1.31
33	BA	2340	A	C8-N7	7.55	1.36	1.31
1	AA	874	A	C8-N7	7.54	1.36	1.31
1	AA	879	A	C8-N7	7.54	1.36	1.31
33	BA	1326	A	C8-N7	7.54	1.36	1.31
33	BA	1426	A	C8-N7	7.54	1.36	1.31
33	BA	1533	A	C8-N7	7.54	1.36	1.31
1	AA	617	A	C8-N7	7.54	1.36	1.31
1	AA	659	A	C8-N7	7.54	1.36	1.31
1	AA	1451	A	C8-N7	7.54	1.36	1.31
33	BA	584	A	C8-N7	7.54	1.36	1.31
33	BA	943	A	C8-N7	7.54	1.36	1.31
1	AA	290	A	C8-N7	7.54	1.36	1.31
1	AA	616	A	C8-N7	7.54	1.36	1.31
33	BA	355	A	C8-N7	7.54	1.36	1.31
33	BA	978	A	C8-N7	7.54	1.36	1.31
33	BA	1235	A	C8-N7	7.54	1.36	1.31
33	BA	1588	A	C8-N7	7.54	1.36	1.31
33	BA	1967	A	C8-N7	7.54	1.36	1.31
33	BA	2327	A	C8-N7	7.54	1.36	1.31
33	BA	2619	A	C8-N7	7.54	1.36	1.31
33	BA	2734	A	C8-N7	7.54	1.36	1.31
1	AA	638	A	C8-N7	7.54	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	677	A	C8-N7	7.54	1.36	1.31
33	BA	765	A	C8-N7	7.54	1.36	1.31
33	BA	1405	A	C8-N7	7.54	1.36	1.31
1	AA	140	A	C8-N7	7.54	1.36	1.31
1	AA	532	A	C8-N7	7.54	1.36	1.31
33	BA	324	A	C8-N7	7.54	1.36	1.31
33	BA	1723	A	C8-N7	7.54	1.36	1.31
33	BA	1929	A	C8-N7	7.54	1.36	1.31
33	BA	2594	A	C8-N7	7.54	1.36	1.31
33	BA	2740	A	C8-N7	7.54	1.36	1.31
1	AA	978	A	C8-N7	7.54	1.36	1.31
1	AA	1121	A	C8-N7	7.54	1.36	1.31
21	AX	76	A	C8-N7	7.54	1.36	1.31
33	BA	38	A	C8-N7	7.54	1.36	1.31
33	BA	150	A	C8-N7	7.54	1.36	1.31
33	BA	339	A	C8-N7	7.54	1.36	1.31
33	BA	437	A	C8-N7	7.54	1.36	1.31
33	BA	2762	A	C8-N7	7.54	1.36	1.31
33	BA	2923	A	C8-N7	7.54	1.36	1.31
1	AA	204	A	C8-N7	7.53	1.36	1.31
1	AA	225	A	C8-N7	7.53	1.36	1.31
1	AA	287	A	C8-N7	7.53	1.36	1.31
1	AA	321	A	C8-N7	7.53	1.36	1.31
1	AA	696	A	C8-N7	7.53	1.36	1.31
1	AA	959	A	C8-N7	7.53	1.36	1.31
33	BA	894	A	C8-N7	7.53	1.36	1.31
33	BA	1895	A	C8-N7	7.53	1.36	1.31
33	BA	1918	A	C8-N7	7.53	1.36	1.31
33	BA	2364	A	C8-N7	7.53	1.36	1.31
1	AA	956	A	C8-N7	7.53	1.36	1.31
1	AA	730	A	C8-N7	7.53	1.36	1.31
1	AA	947	A	C8-N7	7.53	1.36	1.31
33	BA	307	A	C8-N7	7.53	1.36	1.31
33	BA	904	A	C8-N7	7.53	1.36	1.31
33	BA	1663	A	C8-N7	7.53	1.36	1.31
33	BA	1957	A	C8-N7	7.53	1.36	1.31
33	BA	2018	A	C8-N7	7.53	1.36	1.31
33	BA	2100	A	C8-N7	7.53	1.36	1.31
33	BA	2216	A	C8-N7	7.53	1.36	1.31
33	BA	2369	A	C8-N7	7.53	1.36	1.31
33	BA	2708	A	C8-N7	7.53	1.36	1.31
1	AA	72	A	C8-N7	7.53	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	592	A	C8-N7	7.53	1.36	1.31
33	BA	683	A	C8-N7	7.53	1.36	1.31
33	BA	2007	A	C8-N7	7.53	1.36	1.31
33	BA	2658	A	C8-N7	7.53	1.36	1.31
1	AA	271	A	C8-N7	7.53	1.36	1.31
1	AA	372	A	C8-N7	7.53	1.36	1.31
33	BA	236	A	C8-N7	7.53	1.36	1.31
33	BA	1982	A	C8-N7	7.53	1.36	1.31
33	BA	2298	A	C8-N7	7.53	1.36	1.31
33	BA	2406	A	C8-N7	7.53	1.36	1.31
33	BA	2440	A	C8-N7	7.53	1.36	1.31
33	BA	21	A	C8-N7	7.53	1.36	1.31
33	BA	71	A	C8-N7	7.53	1.36	1.31
33	BA	231	A	C8-N7	7.53	1.36	1.31
33	BA	475	A	C8-N7	7.53	1.36	1.31
34	BB	113	A	C8-N7	7.53	1.36	1.31
1	AA	768	A	C8-N7	7.52	1.36	1.31
33	BA	947	A	C8-N7	7.52	1.36	1.31
33	BA	1580	A	C8-N7	7.52	1.36	1.31
33	BA	2297	A	C8-N7	7.52	1.36	1.31
33	BA	2869	A	C8-N7	7.52	1.36	1.31
1	AA	234	A	C8-N7	7.52	1.36	1.31
33	BA	225	A	C8-N7	7.52	1.36	1.31
33	BA	530	A	C8-N7	7.52	1.36	1.31
33	BA	1491	A	C8-N7	7.52	1.36	1.31
33	BA	1700	A	C8-N7	7.52	1.36	1.31
33	BA	2315	A	C8-N7	7.52	1.36	1.31
33	BA	2810	A	C8-N7	7.52	1.36	1.31
1	AA	604	A	C8-N7	7.52	1.36	1.31
1	AA	650	A	C8-N7	7.52	1.36	1.31
33	BA	456	A	C8-N7	7.52	1.36	1.31
33	BA	882	A	C8-N7	7.52	1.36	1.31
33	BA	1375	A	C8-N7	7.52	1.36	1.31
33	BA	2339	A	C8-N7	7.52	1.36	1.31
1	AA	1256	A	C8-N7	7.52	1.36	1.31
1	AA	1523	A	C8-N7	7.52	1.36	1.31
33	BA	705	A	C8-N7	7.52	1.36	1.31
33	BA	1036	A	C8-N7	7.52	1.36	1.31
33	BA	1266	A	C8-N7	7.52	1.36	1.31
33	BA	2052	A	C8-N7	7.52	1.36	1.31
33	BA	2532	A	C8-N7	7.52	1.36	1.31
33	BA	2834	A	C8-N7	7.52	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	185	A	C8-N7	7.52	1.36	1.31
33	BA	1194	A	C8-N7	7.52	1.36	1.31
33	BA	1583	A	C8-N7	7.52	1.36	1.31
33	BA	1585	A	C8-N7	7.52	1.36	1.31
33	BA	1989	A	C8-N7	7.52	1.36	1.31
33	BA	2417	A	C8-N7	7.52	1.36	1.31
1	AA	364	A	C8-N7	7.52	1.36	1.31
1	AA	1528	A	C8-N7	7.52	1.36	1.31
33	BA	1981	A	C8-N7	7.52	1.36	1.31
33	BA	2124	A	C8-N7	7.52	1.36	1.31
33	BA	2390	A	C8-N7	7.52	1.36	1.31
34	BB	37	A	C8-N7	7.52	1.36	1.31
1	AA	605	A	C8-N7	7.51	1.36	1.31
1	AA	1147	A	C8-N7	7.51	1.36	1.31
33	BA	500	A	C8-N7	7.51	1.36	1.31
33	BA	600	A	C8-N7	7.51	1.36	1.31
33	BA	889	A	C8-N7	7.51	1.36	1.31
33	BA	1490	A	C8-N7	7.51	1.36	1.31
33	BA	1767	A	C8-N7	7.51	1.36	1.31
33	BA	2047	A	C8-N7	7.51	1.36	1.31
1	AA	630	A	C8-N7	7.51	1.36	1.31
33	BA	176	A	C8-N7	7.51	1.36	1.31
33	BA	428	A	C8-N7	7.51	1.36	1.31
33	BA	486	A	C8-N7	7.51	1.36	1.31
33	BA	653	A	C8-N7	7.51	1.36	1.31
33	BA	1721	A	C8-N7	7.51	1.36	1.31
33	BA	2066	A	C8-N7	7.51	1.36	1.31
1	AA	1248	A	C8-N7	7.51	1.36	1.31
33	BA	10	A	C8-N7	7.51	1.36	1.31
33	BA	436	A	C8-N7	7.51	1.36	1.31
33	BA	1655	A	C8-N7	7.51	1.36	1.31
33	BA	1685	A	C8-N7	7.51	1.36	1.31
33	BA	1760	A	C8-N7	7.51	1.36	1.31
33	BA	2547	A	C8-N7	7.51	1.36	1.31
33	BA	2787	A	C8-N7	7.51	1.36	1.31
1	AA	81	A	C8-N7	7.51	1.36	1.31
1	AA	94	A	C8-N7	7.51	1.36	1.31
33	BA	548	A	C8-N7	7.51	1.36	1.31
33	BA	2006	A	C8-N7	7.51	1.36	1.31
33	BA	2830	A	C8-N7	7.51	1.36	1.31
1	AA	1529	A	C8-N7	7.51	1.36	1.31
33	BA	1243	A	C8-N7	7.51	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2296	A	C8-N7	7.51	1.36	1.31
33	BA	2904	A	C8-N7	7.51	1.36	1.31
1	AA	945	A	C8-N7	7.51	1.36	1.31
1	AA	1197	A	C8-N7	7.51	1.36	1.31
33	BA	194	A	C8-N7	7.51	1.36	1.31
33	BA	268	A	C8-N7	7.51	1.36	1.31
33	BA	376	A	C8-N7	7.51	1.36	1.31
33	BA	1265	A	C8-N7	7.51	1.36	1.31
33	BA	1809	A	C8-N7	7.51	1.36	1.31
33	BA	2571	A	C8-N7	7.51	1.36	1.31
33	BA	2804	A	C8-N7	7.51	1.36	1.31
33	BA	2919	A	C8-N7	7.51	1.36	1.31
1	AA	281	A	C8-N7	7.50	1.36	1.31
1	AA	793	A	C8-N7	7.50	1.36	1.31
33	BA	407	A	C8-N7	7.50	1.36	1.31
33	BA	1357	A	C8-N7	7.50	1.36	1.31
33	BA	2907	A	C8-N7	7.50	1.36	1.31
1	AA	120	A	C8-N7	7.50	1.36	1.31
1	AA	329	A	C8-N7	7.50	1.36	1.31
33	BA	220	A	C8-N7	7.50	1.36	1.31
33	BA	987	A	C8-N7	7.50	1.36	1.31
33	BA	1506	A	C8-N7	7.50	1.36	1.31
33	BA	1553	A	C8-N7	7.50	1.36	1.31
34	BB	44	A	C8-N7	7.50	1.36	1.31
1	AA	512	A	C8-N7	7.50	1.36	1.31
33	BA	84	A	C8-N7	7.50	1.36	1.31
33	BA	622	A	C8-N7	7.50	1.36	1.31
33	BA	2889	A	C8-N7	7.50	1.36	1.31
1	AA	679	A	C8-N7	7.50	1.36	1.31
1	AA	1261	A	C8-N7	7.50	1.36	1.31
33	BA	12	A	C8-N7	7.50	1.36	1.31
33	BA	384	A	C8-N7	7.50	1.36	1.31
33	BA	524	A	C8-N7	7.50	1.36	1.31
33	BA	774	A	C8-N7	7.50	1.36	1.31
33	BA	835	A	C8-N7	7.50	1.36	1.31
33	BA	1132	A	C8-N7	7.50	1.36	1.31
33	BA	1260	A	C8-N7	7.50	1.36	1.31
33	BA	1277	A	C8-N7	7.50	1.36	1.31
33	BA	1517	A	C8-N7	7.50	1.36	1.31
33	BA	2846	A	C8-N7	7.50	1.36	1.31
1	AA	128	A	C8-N7	7.50	1.36	1.31
1	AA	758	A	C8-N7	7.50	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1103	A	C8-N7	7.50	1.36	1.31
33	BA	429	A	C8-N7	7.50	1.36	1.31
33	BA	1404	A	C8-N7	7.50	1.36	1.31
33	BA	1617	A	C8-N7	7.50	1.36	1.31
33	BA	2387	A	C8-N7	7.50	1.36	1.31
1	AA	346	A	C8-N7	7.50	1.36	1.31
1	AA	1348	A	C8-N7	7.50	1.36	1.31
1	AA	12	A	C8-N7	7.49	1.36	1.31
1	AA	61	A	C8-N7	7.49	1.36	1.31
1	AA	107	A	C8-N7	7.49	1.36	1.31
33	BA	41	A	C8-N7	7.49	1.36	1.31
33	BA	519	A	C8-N7	7.49	1.36	1.31
33	BA	1126	A	C8-N7	7.49	1.36	1.31
33	BA	1421	A	C8-N7	7.49	1.36	1.31
33	BA	1556	A	C8-N7	7.49	1.36	1.31
33	BA	1838	A	C8-N7	7.49	1.36	1.31
33	BA	1942	A	C8-N7	7.49	1.36	1.31
33	BA	2338	A	C8-N7	7.49	1.36	1.31
33	BA	2462	A	C8-N7	7.49	1.36	1.31
34	BB	105	A	C8-N7	7.49	1.36	1.31
33	BA	2848	A	C8-N7	7.49	1.36	1.31
33	BA	2851	A	C8-N7	7.49	1.36	1.31
1	AA	381	A	C8-N7	7.49	1.36	1.31
33	BA	537	A	C8-N7	7.49	1.36	1.31
33	BA	893	A	C8-N7	7.49	1.36	1.31
33	BA	970	A	C8-N7	7.49	1.36	1.31
33	BA	1254	A	C8-N7	7.49	1.36	1.31
33	BA	1392	A	C8-N7	7.49	1.36	1.31
33	BA	1745	A	C8-N7	7.49	1.36	1.31
33	BA	1913	A	C8-N7	7.49	1.36	1.31
1	AA	1111	A	C8-N7	7.49	1.36	1.31
33	BA	790	A	C8-N7	7.49	1.36	1.31
33	BA	1615	A	C8-N7	7.49	1.36	1.31
33	BA	1699	A	C8-N7	7.49	1.36	1.31
33	BA	2643	A	C8-N7	7.49	1.36	1.31
33	BA	1197	A	C8-N7	7.49	1.36	1.31
33	BA	1346	A	C8-N7	7.49	1.36	1.31
33	BA	1710	A	C8-N7	7.49	1.36	1.31
1	AA	390	A	C8-N7	7.49	1.36	1.31
1	AA	583	A	C8-N7	7.49	1.36	1.31
1	AA	984	A	C8-N7	7.49	1.36	1.31
33	BA	230	A	C8-N7	7.49	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	574	A	C8-N7	7.49	1.36	1.31
33	BA	265	A	C8-N7	7.48	1.36	1.31
33	BA	1092	A	C8-N7	7.48	1.36	1.31
33	BA	2132	A	C8-N7	7.48	1.36	1.31
33	BA	2349	A	C8-N7	7.48	1.36	1.31
1	AA	333	A	C8-N7	7.48	1.36	1.31
1	AA	475	A	C8-N7	7.48	1.36	1.31
33	BA	1074	A	C8-N7	7.48	1.36	1.31
33	BA	1998	A	C8-N7	7.48	1.36	1.31
33	BA	2570	A	C8-N7	7.48	1.36	1.31
34	BB	51	A	C8-N7	7.48	1.36	1.31
1	AA	55	A	C8-N7	7.48	1.36	1.31
33	BA	326	A	C8-N7	7.48	1.36	1.31
33	BA	330	A	C8-N7	7.48	1.36	1.31
33	BA	619	A	C8-N7	7.48	1.36	1.31
33	BA	724	A	C8-N7	7.48	1.36	1.31
33	BA	746	A	C8-N7	7.48	1.36	1.31
33	BA	769	A	C8-N7	7.48	1.36	1.31
33	BA	1627	A	C8-N7	7.48	1.36	1.31
33	BA	1845	A	C8-N7	7.48	1.36	1.31
33	BA	2191	A	C8-N7	7.48	1.36	1.31
33	BA	2329	A	C8-N7	7.48	1.36	1.31
33	BA	53	A	C8-N7	7.48	1.36	1.31
33	BA	623	A	C8-N7	7.48	1.36	1.31
1	AA	979	A	C8-N7	7.48	1.36	1.31
33	BA	260	A	C8-N7	7.48	1.36	1.31
33	BA	1524	A	C8-N7	7.48	1.36	1.31
33	BA	1541	A	C8-N7	7.48	1.36	1.31
33	BA	1542	A	C8-N7	7.48	1.36	1.31
33	BA	2405	A	C8-N7	7.48	1.36	1.31
33	BA	2924	A	C8-N7	7.48	1.36	1.31
1	AA	1155	A	C8-N7	7.48	1.36	1.31
1	AA	902	A	C8-N7	7.47	1.36	1.31
1	AA	1222	A	C8-N7	7.47	1.36	1.31
1	AA	1403	A	C8-N7	7.47	1.36	1.31
33	BA	1464	A	C8-N7	7.47	1.36	1.31
33	BA	2316	A	C8-N7	7.47	1.36	1.31
33	BA	2662	A	C8-N7	7.47	1.36	1.31
1	AA	1160	A	C8-N7	7.47	1.36	1.31
1	AA	1238	A	C8-N7	7.47	1.36	1.31
33	BA	140	A	C8-N7	7.47	1.36	1.31
33	BA	171	A	C8-N7	7.47	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	616	A	C8-N7	7.47	1.36	1.31
33	BA	1818	A	C8-N7	7.47	1.36	1.31
33	BA	1965	A	C8-N7	7.47	1.36	1.31
33	BA	2779	A	C8-N7	7.47	1.36	1.31
1	AA	1252	A	C8-N7	7.47	1.36	1.31
1	AA	1513	A	C8-N7	7.47	1.36	1.31
1	AA	160	A	C8-N7	7.47	1.36	1.31
1	AA	210	A	C8-N7	7.47	1.36	1.31
1	AA	776	A	C8-N7	7.47	1.36	1.31
1	AA	886	A	C8-N7	7.47	1.36	1.31
33	BA	14	A	C8-N7	7.47	1.36	1.31
33	BA	1608	A	C8-N7	7.47	1.36	1.31
33	BA	2351	A	C8-N7	7.47	1.36	1.31
33	BA	2421	A	C8-N7	7.47	1.36	1.31
33	BA	658	A	C8-N7	7.47	1.36	1.31
1	AA	1463	A	C8-N7	7.47	1.36	1.31
33	BA	1131	A	C8-N7	7.47	1.36	1.31
33	BA	2770	A	C8-N7	7.47	1.36	1.31
1	AA	35	A	C8-N7	7.46	1.36	1.31
1	AA	796	A	C8-N7	7.46	1.36	1.31
1	AA	1206	A	C8-N7	7.46	1.36	1.31
21	AX	70	A	C8-N7	7.46	1.36	1.31
33	BA	828	A	C8-N7	7.46	1.36	1.31
33	BA	1727	A	C8-N7	7.46	1.36	1.31
33	BA	2270	A	C8-N7	7.46	1.36	1.31
33	BA	876	A	C8-N7	7.46	1.36	1.31
33	BA	1802	A	C8-N7	7.46	1.36	1.31
33	BA	2059	A	C8-N7	7.46	1.36	1.31
33	BA	1695	A	C8-N7	7.46	1.36	1.31
33	BA	2148	A	C8-N7	7.46	1.36	1.31
1	AA	919	A	C8-N7	7.46	1.36	1.31
33	BA	391	A	C8-N7	7.46	1.36	1.31
33	BA	753	A	C8-N7	7.46	1.36	1.31
33	BA	974	A	C8-N7	7.46	1.36	1.31
33	BA	1056	A	C8-N7	7.46	1.36	1.31
33	BA	1059	A	C8-N7	7.46	1.36	1.31
33	BA	2464	A	C8-N7	7.46	1.36	1.31
33	BA	1858	A	C8-N7	7.46	1.36	1.31
1	AA	518	A	C8-N7	7.46	1.36	1.31
33	BA	1291	A	C8-N7	7.46	1.36	1.31
1	AA	301	A	C8-N7	7.45	1.36	1.31
1	AA	361	A	C8-N7	7.45	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	460	A	C8-N7	7.45	1.36	1.31
1	AA	711	A	C8-N7	7.45	1.36	1.31
1	AA	1188	A	C8-N7	7.45	1.36	1.31
33	BA	1453	A	C8-N7	7.45	1.36	1.31
33	BA	2302	A	C8-N7	7.45	1.36	1.31
33	BA	2689	A	C8-N7	7.45	1.36	1.31
1	AA	799	A	C8-N7	7.45	1.36	1.31
1	AA	823	A	C8-N7	7.45	1.36	1.31
33	BA	462	A	C8-N7	7.45	1.36	1.31
33	BA	1284	A	C8-N7	7.45	1.36	1.31
33	BA	830	A	C8-N7	7.45	1.36	1.31
33	BA	1149	A	C8-N7	7.45	1.36	1.31
33	BA	1221	A	C8-N7	7.45	1.36	1.31
33	BA	1335	A	C8-N7	7.45	1.36	1.31
33	BA	1648	A	C8-N7	7.45	1.36	1.31
33	BA	1672	A	C8-N7	7.45	1.36	1.31
33	BA	849	A	C8-N7	7.45	1.36	1.31
33	BA	1832	A	C8-N7	7.45	1.36	1.31
33	BA	2080	A	C8-N7	7.45	1.36	1.31
33	BA	2887	A	C8-N7	7.45	1.36	1.31
33	BA	560	A	C8-N7	7.45	1.36	1.31
33	BA	829	A	C8-N7	7.45	1.36	1.31
33	BA	2790	A	C8-N7	7.45	1.36	1.31
1	AA	684	A	C8-N7	7.44	1.36	1.31
33	BA	305	A	C8-N7	7.44	1.36	1.31
33	BA	715	A	C8-N7	7.44	1.36	1.31
33	BA	736	A	C8-N7	7.44	1.36	1.31
33	BA	1073	A	C8-N7	7.44	1.36	1.31
33	BA	1360	A	C8-N7	7.44	1.36	1.31
33	BA	1956	A	C8-N7	7.44	1.36	1.31
33	BA	2060	A	C8-N7	7.44	1.36	1.31
33	BA	2812	A	C8-N7	7.44	1.36	1.31
1	AA	724	A	C8-N7	7.44	1.36	1.31
33	BA	1054	A	C8-N7	7.44	1.36	1.31
33	BA	2027	A	C8-N7	7.44	1.36	1.31
33	BA	2463	A	C8-N7	7.44	1.36	1.31
1	AA	1328	A	C8-N7	7.44	1.36	1.31
33	BA	13	A	C8-N7	7.44	1.36	1.31
33	BA	1100	A	C8-N7	7.44	1.36	1.31
33	BA	1813	A	C8-N7	7.44	1.36	1.31
33	BA	2454	A	C8-N7	7.44	1.36	1.31
33	BA	1042	A	C8-N7	7.44	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	667	A	C8-N7	7.44	1.36	1.31
33	BA	948	A	C8-N7	7.44	1.36	1.31
33	BA	1477	A	C8-N7	7.44	1.36	1.31
1	AA	1143	A	C8-N7	7.44	1.36	1.31
33	BA	1900	A	C8-N7	7.44	1.36	1.31
33	BA	2719	A	C8-N7	7.44	1.36	1.31
33	BA	549	A	C8-N7	7.43	1.36	1.31
34	BB	56	A	C8-N7	7.43	1.36	1.31
1	AA	496	A	C8-N7	7.43	1.36	1.31
1	AA	1031	A	C8-N7	7.43	1.36	1.31
33	BA	449	A	C8-N7	7.43	1.36	1.31
33	BA	1222	A	C8-N7	7.43	1.36	1.31
33	BA	1316	A	C8-N7	7.43	1.36	1.31
1	AA	57	A	C8-N7	7.43	1.36	1.31
1	AA	811	A	C8-N7	7.43	1.36	1.31
1	AA	917	A	C8-N7	7.43	1.36	1.31
1	AA	1383	A	C8-N7	7.43	1.36	1.31
1	AA	1490	A	C8-N7	7.43	1.36	1.31
33	BA	259	A	C8-N7	7.43	1.36	1.31
1	AA	1189	A	C8-N7	7.43	1.36	1.31
1	AA	433	A	C8-N7	7.43	1.36	1.31
1	AA	1284	A	C8-N7	7.43	1.36	1.31
33	BA	469	A	C8-N7	7.43	1.36	1.31
33	BA	1480	A	C8-N7	7.43	1.36	1.31
1	AA	1366	A	C8-N7	7.42	1.36	1.31
33	BA	692	A	C8-N7	7.42	1.36	1.31
33	BA	958	A	C8-N7	7.42	1.36	1.31
33	BA	971	A	C8-N7	7.42	1.36	1.31
33	BA	496	A	C8-N7	7.42	1.36	1.31
33	BA	2228	A	C8-N7	7.42	1.36	1.31
33	BA	1072	A	C8-N7	7.42	1.36	1.31
33	BA	1258	A	C8-N7	7.42	1.36	1.31
33	BA	1312	A	C8-N7	7.42	1.36	1.31
33	BA	2091	A	C8-N7	7.42	1.36	1.31
34	BB	11	A	C8-N7	7.42	1.36	1.31
1	AA	1341	A	C8-N7	7.42	1.36	1.31
33	BA	525	A	C8-N7	7.42	1.36	1.31
33	BA	678	A	C8-N7	7.42	1.36	1.31
33	BA	2205	A	C8-N7	7.42	1.36	1.31
33	BA	2252	A	C8-N7	7.42	1.36	1.31
33	BA	2497	A	C8-N7	7.42	1.36	1.31
33	BA	2511	A	C8-N7	7.42	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	993	A	C8-N7	7.41	1.36	1.31
33	BA	1848	A	C8-N7	7.41	1.36	1.31
33	BA	1174	A	C8-N7	7.41	1.36	1.31
33	BA	2365	A	C8-N7	7.41	1.36	1.31
1	AA	270	A	C8-N7	7.41	1.36	1.31
1	AA	519	A	C8-N7	7.41	1.36	1.31
1	AA	882	A	C8-N7	7.41	1.36	1.31
1	AA	948	A	C8-N7	7.41	1.36	1.31
1	AA	1161	A	C8-N7	7.41	1.36	1.31
33	BA	659	A	C8-N7	7.41	1.36	1.31
33	BA	1536	A	C8-N7	7.41	1.36	1.31
33	BA	2805	A	C8-N7	7.41	1.36	1.31
1	AA	462	A	C8-N7	7.41	1.36	1.31
1	AA	644	A	C8-N7	7.41	1.36	1.31
33	BA	1667	A	C8-N7	7.41	1.36	1.31
33	BA	2200	A	C8-N7	7.41	1.36	1.31
33	BA	2402	A	C8-N7	7.41	1.36	1.31
33	BA	2517	A	C8-N7	7.41	1.36	1.31
33	BA	130	A	C8-N7	7.41	1.36	1.31
33	BA	193	A	C8-N7	7.41	1.36	1.31
33	BA	431	A	C8-N7	7.41	1.36	1.31
1	AA	74	A	C8-N7	7.40	1.36	1.31
1	AA	1297	A	C8-N7	7.40	1.36	1.31
33	BA	258	A	C8-N7	7.40	1.36	1.31
33	BA	2704	A	C8-N7	7.40	1.36	1.31
1	AA	1004	A	C8-N7	7.40	1.36	1.31
33	BA	2381	A	C8-N7	7.40	1.36	1.31
34	BB	43	A	C8-N7	7.40	1.36	1.31
1	AA	844	A	C8-N7	7.40	1.36	1.31
1	AA	1245	A	C8-N7	7.40	1.36	1.31
33	BA	1945	A	C8-N7	7.40	1.36	1.31
33	BA	2303	A	C8-N7	7.40	1.36	1.31
1	AA	397	A	C8-N7	7.40	1.36	1.31
1	AA	555	A	C8-N7	7.40	1.36	1.31
1	AA	1296	A	C8-N7	7.40	1.36	1.31
1	AA	1517	A	C8-N7	7.40	1.36	1.31
33	BA	2661	A	C8-N7	7.40	1.36	1.31
34	BB	20	A	C8-N7	7.40	1.36	1.31
1	AA	1024	A	C8-N7	7.39	1.36	1.31
33	BA	1638	A	C8-N7	7.39	1.36	1.31
33	BA	459	A	C8-N7	7.39	1.36	1.31
1	AA	195	A	C8-N7	7.39	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	964	A	C8-N7	7.39	1.36	1.31
33	BA	353	A	C8-N7	7.39	1.36	1.31
33	BA	690	A	C8-N7	7.39	1.36	1.31
33	BA	1768	A	C8-N7	7.39	1.36	1.31
34	BB	46	A	C8-N7	7.39	1.36	1.31
33	BA	1569	A	C8-N7	7.38	1.36	1.31
33	BA	2560	A	C8-N7	7.38	1.36	1.31
1	AA	1179	A	C8-N7	7.38	1.36	1.31
1	AA	838	A	C8-N7	7.38	1.36	1.31
33	BA	1019	A	C8-N7	7.38	1.36	1.31
33	BA	2831	A	C8-N7	7.38	1.36	1.31
33	BA	1575	A	C8-N7	7.38	1.36	1.31
33	BA	156	A	C8-N7	7.38	1.36	1.31
1	AA	1493	A	C8-N7	7.38	1.36	1.31
1	AA	727	A	C8-N7	7.37	1.36	1.31
33	BA	1253	A	C8-N7	7.37	1.36	1.31
33	BA	1096	A	C8-N7	7.37	1.36	1.31
33	BA	1562	A	C8-N7	7.37	1.36	1.31
33	BA	689	A	C8-N7	7.37	1.36	1.31
33	BA	1485	A	C8-N7	7.37	1.36	1.31
33	BA	1831	A	C8-N7	7.37	1.36	1.31
33	BA	2043	A	C8-N7	7.37	1.36	1.31
1	AA	1016	A	C8-N7	7.36	1.36	1.31
1	AA	1112	A	C8-N7	7.36	1.36	1.31
33	BA	1778	A	C8-N7	7.36	1.36	1.31
33	BA	2117	A	C8-N7	7.36	1.36	1.31
33	BA	2227	A	C8-N7	7.36	1.36	1.31
1	AA	918	A	C8-N7	7.36	1.36	1.31
1	AA	161	A	C8-N7	7.36	1.36	1.31
1	AA	1384	A	C8-N7	7.36	1.36	1.31
33	BA	1653	A	C8-N7	7.36	1.36	1.31
33	BA	2794	A	C8-N7	7.36	1.36	1.31
1	AA	337	A	C8-N7	7.35	1.36	1.31
33	BA	656	A	C8-N7	7.35	1.36	1.31
33	BA	343	A	C8-N7	7.35	1.36	1.31
33	BA	1047	A	C8-N7	7.35	1.36	1.31
33	BA	1680	A	C8-N7	7.35	1.36	1.31
33	BA	1877	A	C8-N7	7.35	1.36	1.31
33	BA	1027	A	C8-N7	7.35	1.36	1.31
1	AA	969	A	C8-N7	7.34	1.36	1.31
1	AA	649	A	C8-N7	7.34	1.36	1.31
1	AA	1294	A	C8-N7	7.34	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	870	A	C8-N7	7.34	1.36	1.31
33	BA	275	A	C8-N7	7.34	1.36	1.31
33	BA	1461	A	C8-N7	7.34	1.36	1.31
33	BA	1776	A	C8-N7	7.34	1.36	1.31
33	BA	1999	A	C8-N7	7.34	1.36	1.31
33	BA	2694	A	C8-N7	7.34	1.36	1.31
21	AX	9	A	C8-N7	7.34	1.36	1.31
1	AA	114	A	C8-N7	7.33	1.36	1.31
1	AA	913	A	C8-N7	7.33	1.36	1.31
33	BA	517	A	C8-N7	7.33	1.36	1.31
33	BA	1888	A	C8-N7	7.33	1.36	1.31
33	BA	2616	A	C8-N7	7.33	1.36	1.31
33	BA	1581	A	C8-N7	7.33	1.36	1.31
33	BA	2827	A	C8-N7	7.33	1.36	1.31
33	BA	108	A	C8-N7	7.33	1.36	1.31
33	BA	1103	A	C8-N7	7.33	1.36	1.31
33	BA	956	A	C8-N7	7.33	1.36	1.31
1	AA	548	A	C8-N7	7.33	1.36	1.31
33	BA	2163	A	C8-N7	7.33	1.36	1.31
1	AA	335	A	C8-N7	7.32	1.36	1.31
33	BA	1606	A	C8-N7	7.32	1.36	1.31
33	BA	578	A	C8-N7	7.32	1.36	1.31
1	AA	705	A	C8-N7	7.32	1.36	1.31
34	BB	13	A	C8-N7	7.32	1.36	1.31
21	AX	24	A	C8-N7	7.32	1.36	1.31
33	BA	868	A	C8-N7	7.32	1.36	1.31
33	BA	2663	A	C8-N7	7.32	1.36	1.31
1	AA	883	A	C8-N7	7.31	1.36	1.31
1	AA	1442	A	C8-N7	7.31	1.36	1.31
33	BA	2436	A	C8-N7	7.31	1.36	1.31
1	AA	993	A	C8-N7	7.30	1.36	1.31
33	BA	1190	A	C8-N7	7.30	1.36	1.31
33	BA	2026	A	C8-N7	7.30	1.36	1.31
33	BA	1520	A	C8-N7	7.29	1.36	1.31
33	BA	518	A	C8-N7	7.29	1.36	1.31
1	AA	790	A	C8-N7	7.29	1.36	1.31
1	AA	1272	A	C8-N7	7.29	1.36	1.31
1	AA	1288	A	C8-N7	7.29	1.36	1.31
33	BA	2862	A	C8-N7	7.29	1.36	1.31
33	BA	390	A	C8-N7	7.28	1.36	1.31
33	BA	117	A	C8-N7	7.28	1.36	1.31
33	BA	2143	A	C8-N7	7.28	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1619	A	C8-N7	7.28	1.36	1.31
33	BA	2123	A	C8-N7	7.28	1.36	1.31
34	BB	97	A	C8-N7	7.28	1.36	1.31
1	AA	875	A	C8-N7	7.27	1.36	1.31
1	AA	1166	A	C8-N7	7.27	1.36	1.31
33	BA	1709	A	C8-N7	7.27	1.36	1.31
33	BA	1816	A	C8-N7	7.27	1.36	1.31
1	AA	996	A	C8-N7	7.26	1.36	1.31
33	BA	2044	A	C8-N7	7.26	1.36	1.31
1	AA	572	A	C8-N7	7.26	1.36	1.31
1	AA	987	A	C8-N7	7.26	1.36	1.31
1	AA	1234	A	C8-N7	7.26	1.36	1.31
33	BA	90	A	C8-N7	7.26	1.36	1.31
33	BA	910	A	C8-N7	7.26	1.36	1.31
33	BA	913	A	C8-N7	7.26	1.36	1.31
33	BA	551	A	C8-N7	7.25	1.36	1.31
33	BA	2441	A	C8-N7	7.25	1.36	1.31
33	BA	56	A	C8-N7	7.25	1.36	1.31
33	BA	95	A	C8-N7	7.25	1.36	1.31
1	AA	1065	A	C8-N7	7.25	1.36	1.31
33	BA	2395	A	C8-N7	7.24	1.36	1.31
33	BA	722	A	C8-N7	7.24	1.36	1.31
33	BA	1442	A	C8-N7	7.24	1.36	1.31
33	BA	1928	A	C8-N7	7.24	1.36	1.31
1	AA	1315	A	C8-N7	7.24	1.36	1.31
33	BA	1901	A	C8-N7	7.24	1.36	1.31
33	BA	2844	A	C8-N7	7.24	1.36	1.31
33	BA	226	A	C8-N7	7.23	1.36	1.31
33	BA	634	A	C8-N7	7.23	1.36	1.31
33	BA	2735	A	C8-N7	7.23	1.36	1.31
1	AA	76	A	C8-N7	7.22	1.36	1.31
33	BA	1075	A	C8-N7	7.22	1.36	1.31
33	BA	1620	A	C8-N7	7.22	1.36	1.31
33	BA	2786	A	C8-N7	7.22	1.36	1.31
33	BA	2358	A	C8-N7	7.22	1.36	1.31
33	BA	254	A	C8-N7	7.21	1.36	1.31
33	BA	2106	A	C8-N7	7.21	1.36	1.31
33	BA	2459	A	C8-N7	7.21	1.36	1.31
1	AA	911	A	C8-N7	7.20	1.36	1.31
33	BA	2164	A	C8-N7	7.20	1.36	1.31
33	BA	1393	A	C8-N7	7.20	1.36	1.31
1	AA	1427	A	C8-N7	7.19	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2202	A	C8-N7	7.19	1.36	1.31
33	BA	2111	A	C8-N7	7.18	1.36	1.31
1	AA	933	A	C8-N7	7.18	1.36	1.31
33	BA	630	A	C8-N7	7.18	1.36	1.31
33	BA	2468	A	C8-N7	7.18	1.36	1.31
1	AA	1478	A	C8-N7	7.17	1.36	1.31
33	BA	2176	A	C8-N7	7.17	1.36	1.31
33	BA	1714	A	C8-N7	7.17	1.36	1.31
33	BA	559	A	C8-N7	7.16	1.36	1.31
33	BA	661	A	C8-N7	7.16	1.36	1.31
33	BA	538	A	C8-N7	7.15	1.36	1.31
33	BA	1094	A	C8-N7	7.15	1.36	1.31
33	BA	1691	A	C8-N7	7.14	1.36	1.31
33	BA	866	A	C8-N7	7.13	1.36	1.31
33	BA	752	A	C8-N7	7.12	1.36	1.31
33	BA	52	A	C8-N7	7.10	1.36	1.31
1	AA	1308	A	C8-N7	7.09	1.36	1.31
33	BA	1820	A	C8-N7	7.09	1.36	1.31
33	BA	1839	A	C8-N7	7.08	1.36	1.31
33	BA	1691	A	N3-C4	7.08	1.39	1.34
33	BA	1134	A	N3-C4	7.05	1.39	1.34
33	BA	2691	A	C8-N7	7.05	1.36	1.31
1	AA	405	A	C8-N7	7.04	1.36	1.31
33	BA	168	A	C8-N7	7.01	1.36	1.31
33	BA	673	A	C8-N7	7.00	1.36	1.31
33	BA	527	A	C8-N7	7.00	1.36	1.31
33	BA	935	A	C8-N7	6.96	1.36	1.31
33	BA	1618	A	C8-N7	6.96	1.36	1.31
33	BA	1883	A	C8-N7	6.96	1.36	1.31
1	AA	391	A	C8-N7	6.96	1.36	1.31
1	AA	1308	A	N3-C4	6.96	1.39	1.34
33	BA	2407	A	C8-N7	6.96	1.36	1.31
1	AA	572	A	N3-C4	6.95	1.39	1.34
1	AA	99	A	C8-N7	6.95	1.36	1.31
33	BA	732	A	N3-C4	6.95	1.39	1.34
33	BA	226	A	N3-C4	6.93	1.39	1.34
1	AA	308	A	C8-N7	6.93	1.36	1.31
1	AA	993	A	N3-C4	6.90	1.39	1.34
33	BA	1714	A	N3-C4	6.90	1.39	1.34
33	BA	1006	A	C8-N7	6.88	1.36	1.31
1	AA	405	A	N3-C4	6.85	1.39	1.34
21	AX	37	A	C8-N7	6.85	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	281	A	N3-C4	6.85	1.39	1.34
1	AA	1234	A	N3-C4	6.84	1.39	1.34
33	BA	2786	A	N3-C4	6.82	1.39	1.34
33	BA	1661	A	C8-N7	6.80	1.36	1.31
33	BA	679	A	C8-N7	6.75	1.36	1.31
33	BA	913	A	N3-C4	6.75	1.38	1.34
33	BA	1536	A	N3-C4	6.75	1.38	1.34
33	BA	1134	A	C8-N7	6.75	1.36	1.31
1	AA	1278	A	C8-N7	6.74	1.36	1.31
1	AA	1026	A	C8-N7	6.74	1.36	1.31
1	AA	114	A	N3-C4	6.73	1.38	1.34
33	BA	2402	A	N3-C4	6.73	1.38	1.34
33	BA	1885	A	N3-C4	6.72	1.38	1.34
33	BA	326	A	N3-C4	6.72	1.38	1.34
33	BA	948	A	N3-C4	6.72	1.38	1.34
33	BA	2885	A	C8-N7	6.72	1.36	1.31
33	BA	1360	A	N3-C4	6.72	1.38	1.34
1	AA	727	A	N3-C4	6.71	1.38	1.34
1	AA	173	A	N3-C4	6.71	1.38	1.34
1	AA	507	A	N3-C4	6.71	1.38	1.34
1	AA	1155	A	N3-C4	6.71	1.38	1.34
33	BA	634	A	N3-C4	6.71	1.38	1.34
1	AA	1298	A	N3-C4	6.71	1.38	1.34
34	BB	99	A	C8-N7	6.70	1.36	1.31
34	BB	11	A	N3-C4	6.70	1.38	1.34
33	BA	438	A	N3-C4	6.70	1.38	1.34
33	BA	1858	A	N3-C4	6.70	1.38	1.34
33	BA	1581	A	N3-C4	6.69	1.38	1.34
34	BB	99	A	N3-C4	6.69	1.38	1.34
33	BA	1710	A	N3-C4	6.69	1.38	1.34
33	BA	2220	A	N3-C4	6.69	1.38	1.34
1	AA	1341	A	N3-C4	6.69	1.38	1.34
1	AA	948	A	N3-C4	6.67	1.38	1.34
34	BB	13	A	N3-C4	6.67	1.38	1.34
1	AA	838	A	N3-C4	6.67	1.38	1.34
1	AA	1143	A	N3-C4	6.67	1.38	1.34
33	BA	1900	A	N3-C4	6.67	1.38	1.34
1	AA	404	A	N3-C4	6.67	1.38	1.34
1	AA	81	A	N3-C4	6.66	1.38	1.34
1	AA	234	A	N3-C4	6.66	1.38	1.34
1	AA	978	A	N3-C4	6.66	1.38	1.34
1	AA	1024	A	N3-C4	6.66	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	61	A	N3-C4	6.66	1.38	1.34
1	AA	74	A	N3-C4	6.66	1.38	1.34
33	BA	2143	A	N3-C4	6.66	1.38	1.34
33	BA	592	A	N3-C4	6.66	1.38	1.34
34	BB	71	A	N3-C4	6.66	1.38	1.34
33	BA	124	A	N3-C4	6.66	1.38	1.34
33	BA	1562	A	N3-C4	6.66	1.38	1.34
33	BA	2844	A	N3-C4	6.66	1.38	1.34
34	BB	64	A	N3-C4	6.66	1.38	1.34
33	BA	44	A	N3-C4	6.65	1.38	1.34
33	BA	1667	A	N3-C4	6.65	1.38	1.34
33	BA	1774	A	N3-C4	6.65	1.38	1.34
33	BA	952	A	N3-C4	6.65	1.38	1.34
1	AA	1327	A	N3-C4	6.65	1.38	1.34
1	AA	397	A	N3-C4	6.64	1.38	1.34
1	AA	793	A	N3-C4	6.64	1.38	1.34
1	AA	1256	A	N3-C4	6.64	1.38	1.34
33	BA	715	A	N3-C4	6.64	1.38	1.34
1	AA	452	A	N3-C4	6.64	1.38	1.34
33	BA	90	A	N3-C4	6.64	1.38	1.34
33	BA	1224	A	N3-C4	6.64	1.38	1.34
33	BA	2027	A	N3-C4	6.64	1.38	1.34
1	AA	1451	A	N3-C4	6.64	1.38	1.34
33	BA	1695	A	N3-C4	6.64	1.38	1.34
33	BA	168	A	N3-C4	6.63	1.38	1.34
33	BA	2349	A	N3-C4	6.63	1.38	1.34
1	AA	945	A	N3-C4	6.63	1.38	1.34
33	BA	41	A	N3-C4	6.63	1.38	1.34
33	BA	2202	A	N3-C4	6.63	1.38	1.34
1	AA	956	A	N3-C4	6.63	1.38	1.34
1	AA	1284	A	N3-C4	6.63	1.38	1.34
21	AX	58	A	N3-C4	6.63	1.38	1.34
33	BA	95	A	N3-C4	6.63	1.38	1.34
1	AA	506	A	N3-C4	6.63	1.38	1.34
1	AA	721	A	N3-C4	6.63	1.38	1.34
33	BA	2532	A	N3-C4	6.63	1.38	1.34
1	AA	372	A	N3-C4	6.63	1.38	1.34
33	BA	1655	A	N3-C4	6.63	1.38	1.34
33	BA	278	A	N3-C4	6.62	1.38	1.34
33	BA	456	A	N3-C4	6.62	1.38	1.34
33	BA	1103	A	N3-C4	6.62	1.38	1.34
33	BA	130	A	N3-C4	6.62	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1357	A	N3-C4	6.62	1.38	1.34
33	BA	2316	A	N3-C4	6.62	1.38	1.34
1	AA	99	A	N3-C4	6.62	1.38	1.34
1	AA	150	A	N3-C4	6.62	1.38	1.34
1	AA	1022	A	N3-C4	6.62	1.38	1.34
33	BA	265	A	N3-C4	6.62	1.38	1.34
33	BA	1491	A	N3-C4	6.62	1.38	1.34
33	BA	1876	A	N3-C4	6.62	1.38	1.34
33	BA	2358	A	N3-C4	6.62	1.38	1.34
1	AA	55	A	N3-C4	6.62	1.38	1.34
33	BA	527	A	N3-C4	6.62	1.38	1.34
33	BA	1243	A	N3-C4	6.62	1.38	1.34
1	AA	1147	A	N3-C4	6.62	1.38	1.34
21	AX	14	A	N3-C4	6.62	1.38	1.34
1	AA	1017	A	N3-C4	6.62	1.38	1.34
33	BA	1490	A	N3-C4	6.62	1.38	1.34
33	BA	1672	A	N3-C4	6.62	1.38	1.34
33	BA	339	A	N3-C4	6.61	1.38	1.34
33	BA	584	A	N3-C4	6.61	1.38	1.34
33	BA	2205	A	N3-C4	6.61	1.38	1.34
1	AA	1490	A	N3-C4	6.61	1.38	1.34
21	AX	70	A	N3-C4	6.61	1.38	1.34
33	BA	500	A	N3-C4	6.61	1.38	1.34
1	AA	151	A	N3-C4	6.61	1.38	1.34
1	AA	423	A	N3-C4	6.61	1.38	1.34
1	AA	541	A	N3-C4	6.61	1.38	1.34
33	BA	1631	A	N3-C4	6.61	1.38	1.34
33	BA	2369	A	N3-C4	6.61	1.38	1.34
1	AA	649	A	N3-C4	6.61	1.38	1.34
1	AA	803	A	N3-C4	6.61	1.38	1.34
1	AA	996	A	N3-C4	6.61	1.38	1.34
1	AA	1004	A	N3-C4	6.61	1.38	1.34
1	AA	1288	A	N3-C4	6.61	1.38	1.34
1	AA	1435	A	N3-C4	6.61	1.38	1.34
33	BA	231	A	N3-C4	6.61	1.38	1.34
33	BA	943	A	N3-C4	6.61	1.38	1.34
33	BA	724	A	N3-C4	6.60	1.38	1.34
33	BA	56	A	N3-C4	6.60	1.38	1.34
34	BB	50	A	N3-C4	6.60	1.38	1.34
33	BA	1126	A	N3-C4	6.60	1.38	1.34
33	BA	2812	A	N3-C4	6.60	1.38	1.34
33	BA	1235	A	N3-C4	6.60	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2111	A	N3-C4	6.60	1.38	1.34
34	BB	18	A	N3-C4	6.60	1.38	1.34
34	BB	51	A	N3-C4	6.60	1.38	1.34
33	BA	412	A	N3-C4	6.60	1.38	1.34
33	BA	462	A	N3-C4	6.60	1.38	1.34
33	BA	1412	A	N3-C4	6.60	1.38	1.34
33	BA	1480	A	N3-C4	6.60	1.38	1.34
33	BA	1654	A	N3-C4	6.60	1.38	1.34
33	BA	307	A	N3-C4	6.60	1.38	1.34
33	BA	1323	A	N3-C4	6.60	1.38	1.34
1	AA	195	A	N3-C4	6.59	1.38	1.34
1	AA	1383	A	N3-C4	6.59	1.38	1.34
33	BA	1483	A	N3-C4	6.59	1.38	1.34
33	BA	2479	A	N3-C4	6.59	1.38	1.34
33	BA	407	A	N3-C4	6.59	1.38	1.34
33	BA	2155	A	N3-C4	6.59	1.38	1.34
1	AA	456	A	N3-C4	6.59	1.38	1.34
1	AA	705	A	N3-C4	6.59	1.38	1.34
1	AA	1222	A	N3-C4	6.59	1.38	1.34
33	BA	526	A	N3-C4	6.59	1.38	1.34
33	BA	1877	A	N3-C4	6.59	1.38	1.34
33	BA	2044	A	N3-C4	6.59	1.38	1.34
1	AA	1509	A	N3-C4	6.59	1.38	1.34
33	BA	470	A	N3-C4	6.59	1.38	1.34
33	BA	1404	A	N3-C4	6.59	1.38	1.34
33	BA	2042	A	N3-C4	6.59	1.38	1.34
1	AA	202	A	N3-C4	6.59	1.38	1.34
1	AA	282	A	N3-C4	6.59	1.38	1.34
33	BA	1942	A	N3-C4	6.59	1.38	1.34
33	BA	2117	A	N3-C4	6.59	1.38	1.34
33	BA	2148	A	N3-C4	6.59	1.38	1.34
33	BA	530	A	N3-C4	6.58	1.38	1.34
33	BA	1346	A	N3-C4	6.58	1.38	1.34
1	AA	12	A	N3-C4	6.58	1.38	1.34
33	BA	1144	A	N3-C4	6.58	1.38	1.34
33	BA	1906	A	N3-C4	6.58	1.38	1.34
33	BA	1965	A	N3-C4	6.58	1.38	1.34
1	AA	321	A	N3-C4	6.58	1.38	1.34
1	AA	1272	A	N3-C4	6.58	1.38	1.34
1	AA	1358	A	N3-C4	6.58	1.38	1.34
33	BA	736	A	N3-C4	6.58	1.38	1.34
33	BA	1398	A	N3-C4	6.58	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2047	A	N3-C4	6.58	1.38	1.34
33	BA	2123	A	N3-C4	6.58	1.38	1.34
33	BA	2252	A	N3-C4	6.58	1.38	1.34
1	AA	287	A	N3-C4	6.58	1.38	1.34
1	AA	474	A	N3-C4	6.58	1.38	1.34
33	BA	2163	A	N3-C4	6.58	1.38	1.34
1	AA	128	A	N3-C4	6.58	1.38	1.34
1	AA	1466	A	N3-C4	6.58	1.38	1.34
33	BA	762	A	N3-C4	6.58	1.38	1.34
33	BA	910	A	N3-C4	6.58	1.38	1.34
33	BA	1663	A	N3-C4	6.58	1.38	1.34
33	BA	1816	A	N3-C4	6.58	1.38	1.34
1	AA	491	A	N3-C4	6.58	1.38	1.34
33	BA	1809	A	N3-C4	6.58	1.38	1.34
33	BA	2030	A	N3-C4	6.58	1.38	1.34
1	AA	62	A	N3-C4	6.58	1.38	1.34
1	AA	94	A	N3-C4	6.58	1.38	1.34
33	BA	1453	A	N3-C4	6.58	1.38	1.34
1	AA	658	A	N3-C4	6.57	1.38	1.34
21	AX	24	A	N3-C4	6.57	1.38	1.34
21	AX	76	A	N3-C4	6.57	1.38	1.34
33	BA	52	A	N3-C4	6.57	1.38	1.34
33	BA	513	A	C8-N7	6.57	1.36	1.31
33	BA	1845	A	N3-C4	6.57	1.38	1.34
33	BA	2176	A	N3-C4	6.57	1.38	1.34
33	BA	2405	A	N3-C4	6.57	1.38	1.34
33	BA	2907	A	N3-C4	6.57	1.38	1.34
1	AA	875	A	N3-C4	6.57	1.38	1.34
33	BA	102	A	N3-C4	6.57	1.38	1.34
1	AA	361	A	N3-C4	6.57	1.38	1.34
1	AA	617	A	N3-C4	6.57	1.38	1.34
1	AA	677	A	N3-C4	6.57	1.38	1.34
33	BA	616	A	N3-C4	6.57	1.38	1.34
33	BA	1905	A	N3-C4	6.57	1.38	1.34
33	BA	2869	A	N3-C4	6.57	1.38	1.34
34	BB	102	A	N3-C4	6.57	1.38	1.34
33	BA	1005	A	N3-C4	6.57	1.38	1.34
33	BA	1713	A	N3-C4	6.57	1.38	1.34
33	BA	2165	A	N3-C4	6.57	1.38	1.34
33	BA	2900	A	N3-C4	6.57	1.38	1.34
1	AA	1103	A	N3-C4	6.57	1.38	1.34
33	BA	373	A	N3-C4	6.57	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	437	A	N3-C4	6.57	1.38	1.34
33	BA	689	A	N3-C4	6.57	1.38	1.34
33	BA	1222	A	N3-C4	6.57	1.38	1.34
1	AA	31	A	N3-C4	6.57	1.38	1.34
1	AA	542	A	N3-C4	6.57	1.38	1.34
1	AA	870	A	N3-C4	6.57	1.38	1.34
1	AA	1092	A	N3-C4	6.57	1.38	1.34
1	AA	1178	A	N3-C4	6.57	1.38	1.34
33	BA	330	A	N3-C4	6.57	1.38	1.34
33	BA	1788	A	N3-C4	6.57	1.38	1.34
33	BA	2916	A	N3-C4	6.57	1.38	1.34
1	AA	1488	A	N3-C4	6.56	1.38	1.34
33	BA	2339	A	N3-C4	6.56	1.38	1.34
1	AA	1386	A	N3-C4	6.56	1.38	1.34
33	BA	679	A	N3-C4	6.56	1.38	1.34
33	BA	922	A	N3-C4	6.56	1.38	1.34
33	BA	1210	A	N3-C4	6.56	1.38	1.34
33	BA	1585	A	N3-C4	6.56	1.38	1.34
33	BA	1760	A	N3-C4	6.56	1.38	1.34
33	BA	1768	A	N3-C4	6.56	1.38	1.34
33	BA	2043	A	N3-C4	6.56	1.38	1.34
33	BA	2106	A	N3-C4	6.56	1.38	1.34
33	BA	2505	A	N3-C4	6.56	1.38	1.34
33	BA	2735	A	N3-C4	6.56	1.38	1.34
33	BA	2831	A	N3-C4	6.56	1.38	1.34
1	AA	346	A	N3-C4	6.56	1.38	1.34
21	AX	9	A	N3-C4	6.56	1.38	1.34
33	BA	449	A	N3-C4	6.56	1.38	1.34
33	BA	459	A	N3-C4	6.56	1.38	1.34
33	BA	1025	A	N3-C4	6.56	1.38	1.34
33	BA	1056	A	N3-C4	6.56	1.38	1.34
33	BA	2049	A	N3-C4	6.56	1.38	1.34
33	BA	2407	A	N3-C4	6.56	1.38	1.34
33	BA	2662	A	N3-C4	6.56	1.38	1.34
33	BA	2862	A	N3-C4	6.56	1.38	1.34
1	AA	433	A	N3-C4	6.56	1.38	1.34
1	AA	638	A	N3-C4	6.56	1.38	1.34
1	AA	757	A	N3-C4	6.56	1.38	1.34
1	AA	1128	A	N3-C4	6.56	1.38	1.34
33	BA	202	A	N3-C4	6.56	1.38	1.34
33	BA	345	A	N3-C4	6.56	1.38	1.34
33	BA	699	A	N3-C4	6.56	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	958	A	N3-C4	6.56	1.38	1.34
33	BA	1532	A	N3-C4	6.56	1.38	1.34
33	BA	1638	A	N3-C4	6.56	1.38	1.34
1	AA	459	A	N3-C4	6.56	1.38	1.34
1	AA	790	A	N3-C4	6.56	1.38	1.34
33	BA	987	A	N3-C4	6.56	1.38	1.34
33	BA	2827	A	N3-C4	6.56	1.38	1.34
1	AA	189	A	N3-C4	6.55	1.38	1.34
1	AA	1271	A	N3-C4	6.55	1.38	1.34
33	BA	108	A	N3-C4	6.55	1.38	1.34
33	BA	333	A	N3-C4	6.55	1.38	1.34
33	BA	1188	A	N3-C4	6.55	1.38	1.34
33	BA	1797	A	N3-C4	6.55	1.38	1.34
33	BA	2307	A	N3-C4	6.55	1.38	1.34
33	BA	2351	A	N3-C4	6.55	1.38	1.34
33	BA	2441	A	N3-C4	6.55	1.38	1.34
33	BA	2627	A	C8-N7	6.55	1.36	1.31
33	BA	2902	A	N3-C4	6.55	1.38	1.34
1	AA	1320	A	N3-C4	6.55	1.38	1.34
33	BA	390	A	N3-C4	6.55	1.38	1.34
33	BA	896	A	N3-C4	6.55	1.38	1.34
33	BA	1019	A	N3-C4	6.55	1.38	1.34
33	BA	2924	A	N3-C4	6.55	1.38	1.34
1	AA	160	A	N3-C4	6.55	1.38	1.34
1	AA	364	A	N3-C4	6.55	1.38	1.34
1	AA	504	A	N3-C4	6.55	1.38	1.34
1	AA	987	A	N3-C4	6.55	1.38	1.34
33	BA	12	A	N3-C4	6.55	1.38	1.34
33	BA	1888	A	N3-C4	6.55	1.38	1.34
33	BA	2315	A	N3-C4	6.55	1.38	1.34
33	BA	2459	A	N3-C4	6.55	1.38	1.34
1	AA	240	A	N3-C4	6.55	1.38	1.34
1	AA	919	A	N3-C4	6.55	1.38	1.34
1	AA	1028	A	N3-C4	6.55	1.38	1.34
33	BA	1142	A	N3-C4	6.55	1.38	1.34
33	BA	1194	A	N3-C4	6.55	1.38	1.34
33	BA	1685	A	N3-C4	6.55	1.38	1.34
33	BA	1838	A	N3-C4	6.55	1.38	1.34
1	AA	501	A	N3-C4	6.55	1.38	1.34
33	BA	1197	A	N3-C4	6.55	1.38	1.34
33	BA	2100	A	N3-C4	6.55	1.38	1.34
33	BA	2700	A	N3-C4	6.55	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2830	A	N3-C4	6.55	1.38	1.34
1	AA	886	A	N3-C4	6.55	1.38	1.34
1	AA	1205	A	N3-C4	6.55	1.38	1.34
33	BA	166	A	N3-C4	6.55	1.38	1.34
33	BA	517	A	N3-C4	6.55	1.38	1.34
33	BA	1100	A	N3-C4	6.55	1.38	1.34
33	BA	1130	A	N3-C4	6.55	1.38	1.34
33	BA	2083	A	N3-C4	6.55	1.38	1.34
33	BA	2421	A	N3-C4	6.55	1.38	1.34
33	BA	2461	A	N3-C4	6.55	1.38	1.34
33	BA	2571	A	N3-C4	6.55	1.38	1.34
33	BA	2908	A	N3-C4	6.55	1.38	1.34
34	BB	46	A	N3-C4	6.55	1.38	1.34
1	AA	1245	A	N3-C4	6.54	1.38	1.34
33	BA	260	A	N3-C4	6.54	1.38	1.34
33	BA	2754	A	N3-C4	6.54	1.38	1.34
1	AA	120	A	N3-C4	6.54	1.38	1.34
1	AA	831	A	N3-C4	6.54	1.38	1.34
1	AA	882	A	N3-C4	6.54	1.38	1.34
1	AA	1252	A	N3-C4	6.54	1.38	1.34
33	BA	2595	A	N3-C4	6.54	1.38	1.34
1	AA	415	A	N3-C4	6.54	1.38	1.34
1	AA	548	A	N3-C4	6.54	1.38	1.34
1	AA	618	A	N3-C4	6.54	1.38	1.34
1	AA	799	A	N3-C4	6.54	1.38	1.34
1	AA	1349	A	N3-C4	6.54	1.38	1.34
33	BA	73	A	N3-C4	6.54	1.38	1.34
33	BA	247	A	N3-C4	6.54	1.38	1.34
33	BA	548	A	N3-C4	6.54	1.38	1.34
33	BA	1116	A	N3-C4	6.54	1.38	1.34
33	BA	1580	A	N3-C4	6.54	1.38	1.34
1	AA	266	A	N3-C4	6.54	1.38	1.34
33	BA	1036	A	N3-C4	6.54	1.38	1.34
33	BA	1579	A	N3-C4	6.54	1.38	1.34
33	BA	2365	A	N3-C4	6.54	1.38	1.34
33	BA	2440	A	N3-C4	6.54	1.38	1.34
1	AA	204	A	N3-C4	6.54	1.38	1.34
1	AA	225	A	N3-C4	6.54	1.38	1.34
1	AA	801	A	N3-C4	6.54	1.38	1.34
1	AA	824	A	N3-C4	6.54	1.38	1.34
21	AX	41	A	N3-C4	6.54	1.38	1.34
21	AX	44	A	N3-C4	6.54	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	652	A	N3-C4	6.54	1.38	1.34
33	BA	1092	A	N3-C4	6.54	1.38	1.34
33	BA	1190	A	N3-C4	6.54	1.38	1.34
33	BA	1617	A	N3-C4	6.54	1.38	1.34
33	BA	2338	A	N3-C4	6.54	1.38	1.34
33	BA	2560	A	N3-C4	6.54	1.38	1.34
1	AA	140	A	N3-C4	6.54	1.38	1.34
1	AA	715	A	N3-C4	6.54	1.38	1.34
33	BA	618	A	N3-C4	6.54	1.38	1.34
1	AA	519	A	N3-C4	6.54	1.38	1.34
1	AA	828	A	N3-C4	6.54	1.38	1.34
1	AA	1315	A	N3-C4	6.54	1.38	1.34
33	BA	21	A	N3-C4	6.54	1.38	1.34
33	BA	525	A	N3-C4	6.54	1.38	1.34
33	BA	1097	A	N3-C4	6.54	1.38	1.34
1	AA	281	A	N3-C4	6.53	1.38	1.34
1	AA	1502	A	N3-C4	6.53	1.38	1.34
33	BA	956	A	N3-C4	6.53	1.38	1.34
33	BA	1175	A	N3-C4	6.53	1.38	1.34
1	AA	53	A	N3-C4	6.53	1.38	1.34
33	BA	637	A	N3-C4	6.53	1.38	1.34
33	BA	2668	A	N3-C4	6.53	1.38	1.34
1	AA	917	A	N3-C4	6.53	1.38	1.34
1	AA	1140	A	N3-C4	6.53	1.38	1.34
1	AA	1266	A	N3-C4	6.53	1.38	1.34
1	AA	1289	A	N3-C4	6.53	1.38	1.34
33	BA	6	A	N3-C4	6.53	1.38	1.34
33	BA	185	A	N3-C4	6.53	1.38	1.34
33	BA	206	A	N3-C4	6.53	1.38	1.34
33	BA	268	A	N3-C4	6.53	1.38	1.34
33	BA	2152	A	N3-C4	6.53	1.38	1.34
1	AA	72	A	N3-C4	6.53	1.38	1.34
1	AA	1054	A	N3-C4	6.53	1.38	1.34
33	BA	752	A	N3-C4	6.53	1.38	1.34
33	BA	1113	A	N3-C4	6.53	1.38	1.34
33	BA	2329	A	N3-C4	6.53	1.38	1.34
1	AA	270	A	N3-C4	6.53	1.38	1.34
1	AA	616	A	N3-C4	6.53	1.38	1.34
1	AA	1328	A	N3-C4	6.53	1.38	1.34
33	BA	1392	A	N3-C4	6.53	1.38	1.34
33	BA	1627	A	N3-C4	6.53	1.38	1.34
1	AA	844	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	1048	A	N3-C4	6.53	1.38	1.34
1	AA	1120	A	N3-C4	6.53	1.38	1.34
33	BA	2794	A	N3-C4	6.53	1.38	1.34
1	AA	811	A	N3-C4	6.52	1.38	1.34
1	AA	1065	A	N3-C4	6.52	1.38	1.34
1	AA	1427	A	N3-C4	6.52	1.38	1.34
33	BA	1131	A	N3-C4	6.52	1.38	1.34
34	BB	27	A	N3-C4	6.52	1.38	1.34
1	AA	139	A	N3-C4	6.52	1.38	1.34
1	AA	671	A	N3-C4	6.52	1.38	1.34
33	BA	418	A	N3-C4	6.52	1.38	1.34
33	BA	727	A	N3-C4	6.52	1.38	1.34
33	BA	888	A	N3-C4	6.52	1.38	1.34
33	BA	1084	A	N3-C4	6.52	1.38	1.34
33	BA	2170	A	N3-C4	6.52	1.38	1.34
33	BA	2343	A	N3-C4	6.52	1.38	1.34
33	BA	2875	A	N3-C4	6.52	1.38	1.34
34	BB	39	A	N3-C4	6.52	1.38	1.34
1	AA	1225	A	N3-C4	6.52	1.38	1.34
1	AA	1523	A	N3-C4	6.52	1.38	1.34
1	AA	438	A	N3-C4	6.52	1.38	1.34
1	AA	460	A	N3-C4	6.52	1.38	1.34
1	AA	659	A	N3-C4	6.52	1.38	1.34
1	AA	1417	A	N3-C4	6.52	1.38	1.34
1	AA	1437	A	N3-C4	6.52	1.38	1.34
33	BA	656	A	N3-C4	6.52	1.38	1.34
33	BA	765	A	N3-C4	6.52	1.38	1.34
33	BA	964	A	N3-C4	6.52	1.38	1.34
33	BA	1132	A	N3-C4	6.52	1.38	1.34
33	BA	1393	A	N3-C4	6.52	1.38	1.34
33	BA	1445	A	N3-C4	6.52	1.38	1.34
33	BA	1485	A	N3-C4	6.52	1.38	1.34
33	BA	1727	A	N3-C4	6.52	1.38	1.34
33	BA	1995	A	N3-C4	6.52	1.38	1.34
1	AA	440	A	N3-C4	6.52	1.38	1.34
1	AA	1026	A	N3-C4	6.52	1.38	1.34
1	AA	1180	A	N3-C4	6.52	1.38	1.34
33	BA	61	A	N3-C4	6.52	1.38	1.34
33	BA	224	A	N3-C4	6.52	1.38	1.34
33	BA	314	A	N3-C4	6.52	1.38	1.34
33	BA	324	A	N3-C4	6.52	1.38	1.34
33	BA	1161	A	N3-C4	6.52	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2661	A	N3-C4	6.52	1.38	1.34
33	BA	2845	A	N3-C4	6.52	1.38	1.34
1	AA	902	A	N3-C4	6.52	1.38	1.34
33	BA	1844	A	N3-C4	6.52	1.38	1.34
33	BA	1930	A	N3-C4	6.52	1.38	1.34
33	BA	2071	A	N3-C4	6.52	1.38	1.34
1	AA	129	A	N3-C4	6.51	1.38	1.34
1	AA	290	A	N3-C4	6.51	1.38	1.34
1	AA	344	A	N3-C4	6.51	1.38	1.34
1	AA	1296	A	N3-C4	6.51	1.38	1.34
33	BA	428	A	N3-C4	6.51	1.38	1.34
33	BA	553	A	N3-C4	6.51	1.38	1.34
33	BA	868	A	N3-C4	6.51	1.38	1.34
33	BA	2317	A	N3-C4	6.51	1.38	1.34
33	BA	2390	A	N3-C4	6.51	1.38	1.34
33	BA	2511	A	N3-C4	6.51	1.38	1.34
1	AA	422	A	N3-C4	6.51	1.38	1.34
1	AA	1257	A	N3-C4	6.51	1.38	1.34
33	BA	173	A	N3-C4	6.51	1.38	1.34
33	BA	1499	A	N3-C4	6.51	1.38	1.34
33	BA	1966	A	N3-C4	6.51	1.38	1.34
33	BA	2000	A	N3-C4	6.51	1.38	1.34
1	AA	389	A	N3-C4	6.51	1.38	1.34
33	BA	139	A	N3-C4	6.51	1.38	1.34
33	BA	646	A	N3-C4	6.51	1.38	1.34
33	BA	851	A	N3-C4	6.51	1.38	1.34
33	BA	1094	A	N3-C4	6.51	1.38	1.34
33	BA	1426	A	N3-C4	6.51	1.38	1.34
33	BA	1677	A	N3-C4	6.51	1.38	1.34
1	AA	1031	A	N3-C4	6.51	1.38	1.34
1	AA	1160	A	N3-C4	6.51	1.38	1.34
1	AA	1294	A	N3-C4	6.51	1.38	1.34
1	AA	1503	A	N3-C4	6.51	1.38	1.34
33	BA	236	A	N3-C4	6.51	1.38	1.34
33	BA	302	A	N3-C4	6.51	1.38	1.34
33	BA	705	A	N3-C4	6.51	1.38	1.34
33	BA	1473	A	N3-C4	6.51	1.38	1.34
33	BA	1948	A	N3-C4	6.51	1.38	1.34
1	AA	391	A	N3-C4	6.51	1.38	1.34
33	BA	2500	A	N3-C4	6.51	1.38	1.34
33	BA	2854	A	N3-C4	6.51	1.38	1.34
1	AA	605	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	823	A	N3-C4	6.51	1.38	1.34
1	AA	947	A	N3-C4	6.51	1.38	1.34
1	AA	1369	A	N3-C4	6.51	1.38	1.34
21	AX	23	A	N3-C4	6.51	1.38	1.34
33	BA	219	A	N3-C4	6.51	1.38	1.34
33	BA	391	A	N3-C4	6.51	1.38	1.34
33	BA	477	A	N3-C4	6.51	1.38	1.34
33	BA	876	A	N3-C4	6.51	1.38	1.34
33	BA	1115	A	N3-C4	6.51	1.38	1.34
33	BA	1316	A	N3-C4	6.51	1.38	1.34
33	BA	1361	A	N3-C4	6.51	1.38	1.34
33	BA	1608	A	N3-C4	6.51	1.38	1.34
33	BA	1778	A	N3-C4	6.51	1.38	1.34
33	BA	2782	A	N3-C4	6.51	1.38	1.34
34	BB	114	A	N3-C4	6.51	1.38	1.34
1	AA	439	A	N3-C4	6.50	1.38	1.34
1	AA	500	A	N3-C4	6.50	1.38	1.34
1	AA	382	A	N3-C4	6.50	1.38	1.34
1	AA	913	A	N3-C4	6.50	1.38	1.34
33	BA	1305	A	N3-C4	6.50	1.38	1.34
33	BA	1620	A	N3-C4	6.50	1.38	1.34
33	BA	1941	A	N3-C4	6.50	1.38	1.34
33	BA	2805	A	N3-C4	6.50	1.38	1.34
33	BA	2834	A	N3-C4	6.50	1.38	1.34
1	AA	159	A	N3-C4	6.50	1.38	1.34
1	AA	401	A	N3-C4	6.50	1.38	1.34
1	AA	485	A	N3-C4	6.50	1.38	1.34
33	BA	1516	A	N3-C4	6.50	1.38	1.34
33	BA	1533	A	N3-C4	6.50	1.38	1.34
33	BA	2134	A	N3-C4	6.50	1.38	1.34
33	BA	2216	A	N3-C4	6.50	1.38	1.34
1	AA	522	A	N3-C4	6.50	1.38	1.34
1	AA	771	A	N3-C4	6.50	1.38	1.34
33	BA	133	A	N3-C4	6.50	1.38	1.34
33	BA	561	A	N3-C4	6.50	1.38	1.34
1	AA	1189	A	N3-C4	6.50	1.38	1.34
1	AA	1206	A	N3-C4	6.50	1.38	1.34
33	BA	140	A	N3-C4	6.50	1.38	1.34
33	BA	619	A	N3-C4	6.50	1.38	1.34
33	BA	978	A	N3-C4	6.50	1.38	1.34
33	BA	1008	A	N3-C4	6.50	1.38	1.34
33	BA	1517	A	N3-C4	6.50	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1618	A	N3-C4	6.50	1.38	1.34
33	BA	2480	A	N3-C4	6.50	1.38	1.34
33	BA	2689	A	N3-C4	6.50	1.38	1.34
1	AA	296	A	N3-C4	6.50	1.38	1.34
1	AA	1248	A	N3-C4	6.50	1.38	1.34
33	BA	244	A	N3-C4	6.50	1.38	1.34
33	BA	543	A	N3-C4	6.50	1.38	1.34
33	BA	908	A	N3-C4	6.50	1.38	1.34
33	BA	1073	A	N3-C4	6.50	1.38	1.34
33	BA	1119	A	N3-C4	6.50	1.38	1.34
33	BA	1442	A	N3-C4	6.50	1.38	1.34
33	BA	1575	A	N3-C4	6.50	1.38	1.34
33	BA	2191	A	N3-C4	6.50	1.38	1.34
1	AA	462	A	N3-C4	6.50	1.38	1.34
1	AA	518	A	N3-C4	6.50	1.38	1.34
1	AA	651	A	N3-C4	6.50	1.38	1.34
33	BA	1925	A	N3-C4	6.50	1.38	1.34
33	BA	2826	A	N3-C4	6.50	1.38	1.34
1	AA	34	A	N3-C4	6.49	1.38	1.34
1	AA	650	A	N3-C4	6.49	1.38	1.34
1	AA	1348	A	N3-C4	6.49	1.38	1.34
1	AA	1366	A	N3-C4	6.49	1.38	1.34
33	BA	549	A	N3-C4	6.49	1.38	1.34
33	BA	866	A	N3-C4	6.49	1.38	1.34
33	BA	2464	A	N3-C4	6.49	1.38	1.34
33	BA	2629	A	N3-C4	6.49	1.38	1.34
33	BA	2846	A	N3-C4	6.49	1.38	1.34
33	BA	524	A	N3-C4	6.49	1.38	1.34
33	BA	2089	A	N3-C4	6.49	1.38	1.34
1	AA	1166	A	N3-C4	6.49	1.38	1.34
1	AA	1384	A	N3-C4	6.49	1.38	1.34
1	AA	1493	A	N3-C4	6.49	1.38	1.34
33	BA	782	A	N3-C4	6.49	1.38	1.34
33	BA	1258	A	N3-C4	6.49	1.38	1.34
1	AA	251	A	N3-C4	6.49	1.38	1.34
1	AA	556	A	N3-C4	6.49	1.38	1.34
33	BA	1339	A	N3-C4	6.49	1.38	1.34
33	BA	1556	A	N3-C4	6.49	1.38	1.34
33	BA	1636	A	N3-C4	6.49	1.38	1.34
33	BA	1791	A	N3-C4	6.49	1.38	1.34
33	BA	2686	A	N3-C4	6.49	1.38	1.34
34	BB	55	A	N3-C4	6.49	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BB	56	A	N3-C4	6.49	1.38	1.34
33	BA	774	A	N3-C4	6.49	1.38	1.34
33	BA	1244	A	N3-C4	6.49	1.38	1.34
33	BA	1277	A	N3-C4	6.49	1.38	1.34
33	BA	1434	A	N3-C4	6.49	1.38	1.34
33	BA	1709	A	N3-C4	6.49	1.38	1.34
33	BA	2436	A	N3-C4	6.49	1.38	1.34
33	BA	2740	A	N3-C4	6.49	1.38	1.34
1	AA	254	A	N3-C4	6.49	1.38	1.34
1	AA	569	A	N3-C4	6.49	1.38	1.34
33	BA	318	A	N3-C4	6.49	1.38	1.34
33	BA	322	A	N3-C4	6.49	1.38	1.34
33	BA	329	A	N3-C4	6.49	1.38	1.34
33	BA	494	A	N3-C4	6.49	1.38	1.34
33	BA	683	A	N3-C4	6.49	1.38	1.34
33	BA	692	A	N3-C4	6.49	1.38	1.34
33	BA	702	A	N3-C4	6.49	1.38	1.34
33	BA	1149	A	N3-C4	6.49	1.38	1.34
33	BA	1555	A	N3-C4	6.49	1.38	1.34
33	BA	1593	A	N3-C4	6.49	1.38	1.34
33	BA	1679	A	N3-C4	6.49	1.38	1.34
33	BA	1700	A	N3-C4	6.49	1.38	1.34
33	BA	1919	A	N3-C4	6.49	1.38	1.34
33	BA	2381	A	N3-C4	6.49	1.38	1.34
33	BA	2542	A	N3-C4	6.49	1.38	1.34
1	AA	777	A	N3-C4	6.48	1.38	1.34
1	AA	899	A	N3-C4	6.48	1.38	1.34
1	AA	1121	A	N3-C4	6.48	1.38	1.34
33	BA	1006	A	N3-C4	6.48	1.38	1.34
33	BA	1066	A	N3-C4	6.48	1.38	1.34
33	BA	1202	A	N3-C4	6.48	1.38	1.34
33	BA	1423	A	N3-C4	6.48	1.38	1.34
33	BA	1534	A	N3-C4	6.48	1.38	1.34
33	BA	2254	A	N3-C4	6.48	1.38	1.34
33	BA	2790	A	N3-C4	6.48	1.38	1.34
1	AA	1512	A	N3-C4	6.48	1.38	1.34
33	BA	974	A	N3-C4	6.48	1.38	1.34
33	BA	1123	A	N3-C4	6.48	1.38	1.34
33	BA	1253	A	N3-C4	6.48	1.38	1.34
1	AA	178	A	N3-C4	6.48	1.38	1.34
1	AA	496	A	N3-C4	6.48	1.38	1.34
1	AA	704	A	N3-C4	6.48	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	713	A	N3-C4	6.48	1.38	1.34
1	AA	883	A	N3-C4	6.48	1.38	1.34
1	AA	1014	A	N3-C4	6.48	1.38	1.34
33	BA	14	A	N3-C4	6.48	1.38	1.34
33	BA	971	A	N3-C4	6.48	1.38	1.34
33	BA	1233	A	N3-C4	6.48	1.38	1.34
33	BA	1312	A	N3-C4	6.48	1.38	1.34
33	BA	2091	A	N3-C4	6.48	1.38	1.34
33	BA	2497	A	N3-C4	6.48	1.38	1.34
33	BA	2762	A	N3-C4	6.48	1.38	1.34
1	AA	985	A	N3-C4	6.48	1.38	1.34
1	AA	1238	A	N3-C4	6.48	1.38	1.34
33	BA	91	A	N3-C4	6.48	1.38	1.34
33	BA	222	A	N3-C4	6.48	1.38	1.34
33	BA	722	A	N3-C4	6.48	1.38	1.34
33	BA	1075	A	N3-C4	6.48	1.38	1.34
33	BA	1286	A	N3-C4	6.48	1.38	1.34
33	BA	1540	A	N3-C4	6.48	1.38	1.34
33	BA	1895	A	N3-C4	6.48	1.38	1.34
33	BA	1913	A	N3-C4	6.48	1.38	1.34
33	BA	2463	A	N3-C4	6.48	1.38	1.34
33	BA	2482	A	N3-C4	6.48	1.38	1.34
1	AA	532	A	N3-C4	6.48	1.38	1.34
1	AA	762	A	N3-C4	6.48	1.38	1.34
1	AA	775	A	N3-C4	6.48	1.38	1.34
33	BA	475	A	N3-C4	6.48	1.38	1.34
33	BA	1055	A	N3-C4	6.48	1.38	1.34
33	BA	1059	A	N3-C4	6.48	1.38	1.34
33	BA	1230	A	N3-C4	6.48	1.38	1.34
34	BB	76	A	N3-C4	6.48	1.38	1.34
1	AA	228	A	N3-C4	6.47	1.38	1.34
1	AA	419	A	N3-C4	6.47	1.38	1.34
1	AA	758	A	N3-C4	6.47	1.38	1.34
1	AA	816	A	N3-C4	6.47	1.38	1.34
33	BA	94	A	N3-C4	6.47	1.38	1.34
33	BA	230	A	N3-C4	6.47	1.38	1.34
33	BA	647	A	N3-C4	6.47	1.38	1.34
33	BA	970	A	N3-C4	6.47	1.38	1.34
33	BA	1260	A	N3-C4	6.47	1.38	1.34
33	BA	2362	A	N3-C4	6.47	1.38	1.34
33	BA	2517	A	N3-C4	6.47	1.38	1.34
33	BA	2691	A	N3-C4	6.47	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2893	A	N3-C4	6.47	1.38	1.34
1	AA	776	A	N3-C4	6.47	1.38	1.34
1	AA	933	A	N3-C4	6.47	1.38	1.34
1	AA	1270	A	N3-C4	6.47	1.38	1.34
33	BA	154	A	N3-C4	6.47	1.38	1.34
33	BA	893	A	N3-C4	6.47	1.38	1.34
33	BA	2658	A	N3-C4	6.47	1.38	1.34
1	AA	67	A	N3-C4	6.47	1.38	1.34
33	BA	110	A	N3-C4	6.47	1.38	1.34
33	BA	1735	A	N3-C4	6.47	1.38	1.34
33	BA	2619	A	N3-C4	6.47	1.38	1.34
33	BA	2778	A	N3-C4	6.47	1.38	1.34
34	BB	97	A	N3-C4	6.47	1.38	1.34
1	AA	314	A	N3-C4	6.47	1.38	1.34
1	AA	367	A	N3-C4	6.47	1.38	1.34
1	AA	457	A	N3-C4	6.47	1.38	1.34
1	AA	644	A	N3-C4	6.47	1.38	1.34
1	AA	711	A	N3-C4	6.47	1.38	1.34
1	AA	1456	A	N3-C4	6.47	1.38	1.34
33	BA	274	A	N3-C4	6.47	1.38	1.34
33	BA	551	A	N3-C4	6.47	1.38	1.34
33	BA	578	A	N3-C4	6.47	1.38	1.34
33	BA	593	A	N3-C4	6.47	1.38	1.34
33	BA	1014	A	N3-C4	6.47	1.38	1.34
33	BA	1375	A	N3-C4	6.47	1.38	1.34
33	BA	1784	A	N3-C4	6.47	1.38	1.34
33	BA	1957	A	N3-C4	6.47	1.38	1.34
33	BA	1989	A	N3-C4	6.47	1.38	1.34
33	BA	2683	A	N3-C4	6.47	1.38	1.34
33	BA	2837	A	N3-C4	6.47	1.38	1.34
1	AA	959	A	N3-C4	6.47	1.38	1.34
1	AA	1442	A	N3-C4	6.47	1.38	1.34
33	BA	1831	A	N3-C4	6.47	1.38	1.34
33	BA	2059	A	N3-C4	6.47	1.38	1.34
1	AA	57	A	N3-C4	6.47	1.38	1.34
1	AA	1102	A	N3-C4	6.47	1.38	1.34
1	AA	1403	A	N3-C4	6.47	1.38	1.34
33	BA	28	A	N3-C4	6.47	1.38	1.34
33	BA	476	A	N3-C4	6.47	1.38	1.34
33	BA	518	A	N3-C4	6.47	1.38	1.34
33	BA	2468	A	N3-C4	6.47	1.38	1.34
33	BA	2526	A	N3-C4	6.47	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2627	A	N3-C4	6.47	1.38	1.34
33	BA	2722	A	N3-C4	6.47	1.38	1.34
33	BA	2885	A	N3-C4	6.47	1.38	1.34
1	AA	918	A	N3-C4	6.46	1.38	1.34
1	AA	1006	A	N3-C4	6.46	1.38	1.34
1	AA	1470	A	N3-C4	6.46	1.38	1.34
33	BA	369	A	N3-C4	6.46	1.38	1.34
33	BA	436	A	N3-C4	6.46	1.38	1.34
33	BA	763	A	N3-C4	6.46	1.38	1.34
33	BA	790	A	N3-C4	6.46	1.38	1.34
33	BA	894	A	N3-C4	6.46	1.38	1.34
33	BA	1381	A	N3-C4	6.46	1.38	1.34
33	BA	1388	A	N3-C4	6.46	1.38	1.34
33	BA	2146	A	N3-C4	6.46	1.38	1.34
1	AA	52	A	N3-C4	6.46	1.38	1.34
1	AA	352	A	N3-C4	6.46	1.38	1.34
1	AA	1419	A	N3-C4	6.46	1.38	1.34
33	BA	258	A	N3-C4	6.46	1.38	1.34
33	BA	1340	A	N3-C4	6.46	1.38	1.34
33	BA	1814	A	N3-C4	6.46	1.38	1.34
33	BA	1815	A	N3-C4	6.46	1.38	1.34
33	BA	2876	A	N3-C4	6.46	1.38	1.34
1	AA	475	A	N3-C4	6.46	1.38	1.34
1	AA	1056	A	N3-C4	6.46	1.38	1.34
1	AA	1425	A	N3-C4	6.46	1.38	1.34
33	BA	723	A	N3-C4	6.46	1.38	1.34
33	BA	889	A	N3-C4	6.46	1.38	1.34
1	AA	333	A	N3-C4	6.46	1.38	1.34
33	BA	275	A	N3-C4	6.46	1.38	1.34
33	BA	661	A	N3-C4	6.46	1.38	1.34
33	BA	1588	A	N3-C4	6.46	1.38	1.34
33	BA	1653	A	N3-C4	6.46	1.38	1.34
33	BA	1945	A	N3-C4	6.46	1.38	1.34
33	BA	2694	A	N3-C4	6.46	1.38	1.34
33	BA	2851	A	N3-C4	6.46	1.38	1.34
33	BA	2904	A	N3-C4	6.46	1.38	1.34
1	AA	1176	A	N3-C4	6.46	1.38	1.34
1	AA	1210	A	N3-C4	6.46	1.38	1.34
33	BA	769	A	N3-C4	6.46	1.38	1.34
33	BA	882	A	N3-C4	6.46	1.38	1.34
33	BA	1789	A	N3-C4	6.46	1.38	1.34
33	BA	1818	A	N3-C4	6.46	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2228	A	N3-C4	6.46	1.38	1.34
33	BA	2270	A	N3-C4	6.46	1.38	1.34
33	BA	2303	A	N3-C4	6.46	1.38	1.34
1	AA	390	A	N3-C4	6.46	1.38	1.34
1	AA	611	A	N3-C4	6.46	1.38	1.34
33	BA	1308	A	N3-C4	6.46	1.38	1.34
33	BA	1813	A	N3-C4	6.46	1.38	1.34
33	BA	2750	A	N3-C4	6.46	1.38	1.34
1	AA	306	A	N3-C4	6.45	1.38	1.34
1	AA	323	A	N3-C4	6.45	1.38	1.34
1	AA	1517	A	N3-C4	6.45	1.38	1.34
33	BA	538	A	N3-C4	6.45	1.38	1.34
33	BA	770	A	N3-C4	6.45	1.38	1.34
33	BA	1465	A	N3-C4	6.45	1.38	1.34
33	BA	1614	A	N3-C4	6.45	1.38	1.34
1	AA	825	A	N3-C4	6.45	1.38	1.34
33	BA	2032	A	N3-C4	6.45	1.38	1.34
33	BA	2124	A	N3-C4	6.45	1.38	1.34
33	BA	2887	A	N3-C4	6.45	1.38	1.34
33	BA	504	A	N3-C4	6.45	1.38	1.34
33	BA	753	A	N3-C4	6.45	1.38	1.34
33	BA	847	A	N3-C4	6.45	1.38	1.34
33	BA	1029	A	N3-C4	6.45	1.38	1.34
33	BA	1042	A	N3-C4	6.45	1.38	1.34
33	BA	1553	A	N3-C4	6.45	1.38	1.34
33	BA	2590	A	N3-C4	6.45	1.38	1.34
1	AA	117	A	N3-C4	6.45	1.38	1.34
1	AA	463	A	N3-C4	6.45	1.38	1.34
1	AA	1297	A	N3-C4	6.45	1.38	1.34
33	BA	171	A	N3-C4	6.45	1.38	1.34
33	BA	1406	A	N3-C4	6.45	1.38	1.34
33	BA	1601	A	N3-C4	6.45	1.38	1.34
33	BA	1767	A	N3-C4	6.45	1.38	1.34
33	BA	2187	A	N3-C4	6.45	1.38	1.34
1	AA	679	A	N3-C4	6.45	1.38	1.34
1	AA	1479	A	N3-C4	6.45	1.38	1.34
1	AA	1513	A	N3-C4	6.45	1.38	1.34
33	BA	176	A	N3-C4	6.45	1.38	1.34
33	BA	1269	A	N3-C4	6.45	1.38	1.34
33	BA	1506	A	N3-C4	6.45	1.38	1.34
1	AA	208	A	N3-C4	6.45	1.38	1.34
1	AA	210	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	672	A	N3-C4	6.45	1.38	1.34
1	AA	928	A	N3-C4	6.45	1.38	1.34
33	BA	13	A	N3-C4	6.45	1.38	1.34
33	BA	429	A	N3-C4	6.45	1.38	1.34
33	BA	1221	A	N3-C4	6.45	1.38	1.34
33	BA	1541	A	N3-C4	6.45	1.38	1.34
33	BA	2507	A	N3-C4	6.45	1.38	1.34
33	BA	2919	A	N3-C4	6.45	1.38	1.34
34	BB	20	A	N3-C4	6.45	1.38	1.34
33	BA	1287	A	N3-C4	6.44	1.38	1.34
33	BA	2298	A	N3-C4	6.44	1.38	1.34
33	BA	2708	A	N3-C4	6.44	1.38	1.34
33	BA	2767	A	N3-C4	6.44	1.38	1.34
1	AA	664	A	N3-C4	6.44	1.38	1.34
1	AA	1278	A	N3-C4	6.44	1.38	1.34
1	AA	1463	A	N3-C4	6.44	1.38	1.34
33	BA	259	A	N3-C4	6.44	1.38	1.34
33	BA	353	A	N3-C4	6.44	1.38	1.34
33	BA	677	A	N3-C4	6.44	1.38	1.34
33	BA	870	A	N3-C4	6.44	1.38	1.34
33	BA	1096	A	N3-C4	6.44	1.38	1.34
33	BA	1961	A	N3-C4	6.44	1.38	1.34
33	BA	2663	A	N3-C4	6.44	1.38	1.34
34	BB	105	A	N3-C4	6.44	1.38	1.34
1	AA	1405	A	N3-C4	6.44	1.38	1.34
33	BA	150	A	N3-C4	6.44	1.38	1.34
33	BA	193	A	N3-C4	6.44	1.38	1.34
33	BA	519	A	N3-C4	6.44	1.38	1.34
33	BA	1027	A	N3-C4	6.44	1.38	1.34
33	BA	1520	A	N3-C4	6.44	1.38	1.34
33	BA	1699	A	N3-C4	6.44	1.38	1.34
33	BA	1743	A	N3-C4	6.44	1.38	1.34
33	BA	2164	A	N3-C4	6.44	1.38	1.34
33	BA	2227	A	N3-C4	6.44	1.38	1.34
1	AA	308	A	N3-C4	6.44	1.38	1.34
1	AA	544	A	N3-C4	6.44	1.38	1.34
1	AA	737	A	N3-C4	6.44	1.38	1.34
1	AA	1455	A	N3-C4	6.44	1.38	1.34
33	BA	1302	A	N3-C4	6.44	1.38	1.34
33	BA	1313	A	N3-C4	6.44	1.38	1.34
33	BA	1314	A	N3-C4	6.44	1.38	1.34
33	BA	1405	A	N3-C4	6.44	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2923	A	N3-C4	6.44	1.38	1.34
34	BB	17	A	N3-C4	6.44	1.38	1.34
1	AA	35	A	N3-C4	6.44	1.38	1.34
1	AA	738	A	N3-C4	6.44	1.38	1.34
1	AA	911	A	N3-C4	6.44	1.38	1.34
1	AA	1200	A	N3-C4	6.44	1.38	1.34
33	BA	10	A	N3-C4	6.44	1.38	1.34
33	BA	690	A	N3-C4	6.44	1.38	1.34
33	BA	1417	A	N3-C4	6.44	1.38	1.34
33	BA	1524	A	N3-C4	6.44	1.38	1.34
33	BA	1776	A	N3-C4	6.44	1.38	1.34
33	BA	1998	A	N3-C4	6.44	1.38	1.34
33	BA	2417	A	N3-C4	6.44	1.38	1.34
1	AA	529	A	N3-C4	6.44	1.38	1.34
1	AA	979	A	N3-C4	6.44	1.38	1.34
33	BA	781	A	N3-C4	6.44	1.38	1.34
34	BB	113	A	N3-C4	6.44	1.38	1.34
1	AA	161	A	N3-C4	6.43	1.38	1.34
1	AA	592	A	N3-C4	6.43	1.38	1.34
1	AA	837	A	N3-C4	6.43	1.38	1.34
1	AA	1434	A	N3-C4	6.43	1.38	1.34
1	AA	1541	A	N3-C4	6.43	1.38	1.34
33	BA	156	A	N3-C4	6.43	1.38	1.34
33	BA	1189	A	N3-C4	6.43	1.38	1.34
1	AA	477	A	N3-C4	6.43	1.38	1.34
1	AA	1161	A	N3-C4	6.43	1.38	1.34
1	AA	1197	A	N3-C4	6.43	1.38	1.34
33	BA	828	A	N3-C4	6.43	1.38	1.34
33	BA	2088	A	N3-C4	6.43	1.38	1.34
33	BA	2327	A	N3-C4	6.43	1.38	1.34
33	BA	2375	A	N3-C4	6.43	1.38	1.34
33	BA	2670	A	N3-C4	6.43	1.38	1.34
33	BA	2719	A	N3-C4	6.43	1.38	1.34
33	BA	38	A	N3-C4	6.43	1.38	1.34
33	BA	1619	A	N3-C4	6.43	1.38	1.34
34	BB	43	A	N3-C4	6.43	1.38	1.34
1	AA	142	A	N3-C4	6.43	1.38	1.34
1	AA	301	A	N3-C4	6.43	1.38	1.34
1	AA	796	A	N3-C4	6.43	1.38	1.34
1	AA	924	A	N3-C4	6.43	1.38	1.34
1	AA	1179	A	N3-C4	6.43	1.38	1.34
33	BA	325	A	N3-C4	6.43	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	421	A	N3-C4	6.43	1.38	1.34
33	BA	600	A	N3-C4	6.43	1.38	1.34
33	BA	758	A	N3-C4	6.43	1.38	1.34
33	BA	1141	A	N3-C4	6.43	1.38	1.34
33	BA	1266	A	N3-C4	6.43	1.38	1.34
33	BA	2078	A	N3-C4	6.43	1.38	1.34
33	BA	2200	A	N3-C4	6.43	1.38	1.34
33	BA	2387	A	N3-C4	6.43	1.38	1.34
33	BA	2793	A	N3-C4	6.43	1.38	1.34
1	AA	335	A	N3-C4	6.43	1.38	1.34
33	BA	537	A	N3-C4	6.43	1.38	1.34
33	BA	904	A	N3-C4	6.43	1.38	1.34
33	BA	1464	A	N3-C4	6.43	1.38	1.34
33	BA	1956	A	N3-C4	6.43	1.38	1.34
33	BA	2256	A	N3-C4	6.43	1.38	1.34
1	AA	371	A	N3-C4	6.43	1.38	1.34
1	AA	791	A	N3-C4	6.43	1.38	1.34
33	BA	210	A	N3-C4	6.43	1.38	1.34
33	BA	513	A	N3-C4	6.43	1.38	1.34
33	BA	572	A	N3-C4	6.43	1.38	1.34
33	BA	653	A	N3-C4	6.43	1.38	1.34
33	BA	1325	A	N3-C4	6.43	1.38	1.34
33	BA	2356	A	N3-C4	6.43	1.38	1.34
33	BA	2364	A	N3-C4	6.43	1.38	1.34
1	AA	512	A	N3-C4	6.42	1.38	1.34
1	AA	925	A	N3-C4	6.42	1.38	1.34
33	BA	207	A	N3-C4	6.42	1.38	1.34
33	BA	1680	A	N3-C4	6.42	1.38	1.34
33	BA	1999	A	N3-C4	6.42	1.38	1.34
33	BA	2383	A	N3-C4	6.42	1.38	1.34
33	BA	376	A	N3-C4	6.42	1.38	1.34
33	BA	2406	A	N3-C4	6.42	1.38	1.34
1	AA	910	A	N3-C4	6.42	1.38	1.34
1	AA	1111	A	N3-C4	6.42	1.38	1.34
33	BA	49	A	N3-C4	6.42	1.38	1.34
33	BA	117	A	N3-C4	6.42	1.38	1.34
33	BA	194	A	N3-C4	6.42	1.38	1.34
33	BA	431	A	N3-C4	6.42	1.38	1.34
33	BA	448	A	N3-C4	6.42	1.38	1.34
1	AA	669	A	N3-C4	6.42	1.38	1.34
1	AA	786	A	N3-C4	6.42	1.38	1.34
33	BA	64	A	N3-C4	6.42	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	486	A	N3-C4	6.42	1.38	1.34
33	BA	507	A	N3-C4	6.42	1.38	1.34
33	BA	1914	A	N3-C4	6.42	1.38	1.34
33	BA	2340	A	N3-C4	6.42	1.38	1.34
1	AA	1213	A	N3-C4	6.42	1.38	1.34
1	AA	1254	A	N3-C4	6.42	1.38	1.34
33	BA	254	A	N3-C4	6.42	1.38	1.34
33	BA	658	A	N3-C4	6.42	1.38	1.34
33	BA	786	A	N3-C4	6.42	1.38	1.34
33	BA	1284	A	N3-C4	6.42	1.38	1.34
33	BA	1504	A	N3-C4	6.42	1.38	1.34
33	BA	1675	A	N3-C4	6.42	1.38	1.34
33	BA	1721	A	N3-C4	6.42	1.38	1.34
33	BA	1883	A	N3-C4	6.42	1.38	1.34
33	BA	2066	A	N3-C4	6.42	1.38	1.34
33	BA	2787	A	N3-C4	6.42	1.38	1.34
1	AA	685	A	N3-C4	6.42	1.38	1.34
1	AA	730	A	N3-C4	6.42	1.38	1.34
1	AA	1283	A	N3-C4	6.42	1.38	1.34
33	BA	144	A	N3-C4	6.42	1.38	1.34
33	BA	199	A	N3-C4	6.42	1.38	1.34
33	BA	999	A	N3-C4	6.42	1.38	1.34
33	BA	1326	A	N3-C4	6.42	1.38	1.34
33	BA	1477	A	N3-C4	6.42	1.38	1.34
33	BA	2777	A	N3-C4	6.42	1.38	1.34
1	AA	171	A	N3-C4	6.41	1.38	1.34
33	BA	384	A	N3-C4	6.41	1.38	1.34
33	BA	388	A	N3-C4	6.41	1.38	1.34
1	AA	1077	A	N3-C4	6.41	1.38	1.34
33	BA	126	A	N3-C4	6.41	1.38	1.34
33	BA	678	A	N3-C4	6.41	1.38	1.34
33	BA	2734	A	N3-C4	6.41	1.38	1.34
1	AA	278	A	N3-C4	6.41	1.38	1.34
1	AA	703	A	N3-C4	6.41	1.38	1.34
1	AA	1090	A	N3-C4	6.41	1.38	1.34
33	BA	469	A	N3-C4	6.41	1.38	1.34
33	BA	1072	A	N3-C4	6.41	1.38	1.34
33	BA	1174	A	N3-C4	6.41	1.38	1.34
33	BA	1254	A	N3-C4	6.41	1.38	1.34
33	BA	1615	A	N3-C4	6.41	1.38	1.34
33	BA	2080	A	N3-C4	6.41	1.38	1.34
33	BA	2119	A	N3-C4	6.41	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1236	A	N3-C4	6.41	1.38	1.34
1	AA	1359	A	N3-C4	6.41	1.38	1.34
1	AA	1478	A	N3-C4	6.41	1.38	1.34
1	AA	1486	A	N3-C4	6.41	1.38	1.34
33	BA	1020	A	N3-C4	6.41	1.38	1.34
33	BA	1054	A	N3-C4	6.41	1.38	1.34
1	AA	1050	A	N3-C4	6.41	1.38	1.34
33	BA	161	A	N3-C4	6.41	1.38	1.34
33	BA	1592	A	N3-C4	6.41	1.38	1.34
1	AA	76	A	N3-C4	6.41	1.38	1.34
1	AA	258	A	N3-C4	6.41	1.38	1.34
1	AA	1259	A	N3-C4	6.41	1.38	1.34
1	AA	1355	A	N3-C4	6.41	1.38	1.34
33	BA	835	A	N3-C4	6.41	1.38	1.34
33	BA	1820	A	N3-C4	6.41	1.38	1.34
33	BA	2018	A	N3-C4	6.41	1.38	1.34
33	BA	2297	A	N3-C4	6.41	1.38	1.34
33	BA	2704	A	N3-C4	6.41	1.38	1.34
33	BA	2769	A	N3-C4	6.41	1.38	1.34
1	AA	203	A	N3-C4	6.40	1.38	1.34
1	AA	337	A	N3-C4	6.40	1.38	1.34
33	BA	305	A	N3-C4	6.40	1.38	1.34
33	BA	547	A	N3-C4	6.40	1.38	1.34
33	BA	575	A	N3-C4	6.40	1.38	1.34
33	BA	867	A	N3-C4	6.40	1.38	1.34
33	BA	2570	A	N3-C4	6.40	1.38	1.34
1	AA	10	A	N3-C4	6.40	1.38	1.34
1	AA	630	A	N3-C4	6.40	1.38	1.34
1	AA	1185	A	N3-C4	6.40	1.38	1.34
33	BA	5	A	N3-C4	6.40	1.38	1.34
33	BA	2330	A	N3-C4	6.40	1.38	1.34
1	AA	190	A	N3-C4	6.40	1.38	1.34
1	AA	232	A	N3-C4	6.40	1.38	1.34
1	AA	1529	A	N3-C4	6.40	1.38	1.34
33	BA	343	A	N3-C4	6.40	1.38	1.34
1	AA	768	A	N3-C4	6.40	1.38	1.34
33	BA	1456	A	N3-C4	6.40	1.38	1.34
1	AA	923	A	N3-C4	6.40	1.38	1.34
33	BA	225	A	N3-C4	6.40	1.38	1.34
33	BA	1061	A	N3-C4	6.40	1.38	1.34
33	BA	1901	A	N3-C4	6.40	1.38	1.34
21	AX	21	A	N3-C4	6.39	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1347	A	N3-C4	6.39	1.38	1.34
1	AA	1372	A	N3-C4	6.39	1.38	1.34
33	BA	53	A	N3-C4	6.39	1.38	1.34
33	BA	740	A	N3-C4	6.39	1.38	1.34
33	BA	1424	A	N3-C4	6.39	1.38	1.34
33	BA	1606	A	N3-C4	6.39	1.38	1.34
33	BA	1967	A	N3-C4	6.39	1.38	1.34
34	BB	44	A	N3-C4	6.39	1.38	1.34
1	AA	975	A	N3-C4	6.39	1.38	1.34
33	BA	1746	A	N3-C4	6.39	1.38	1.34
33	BA	2087	A	N3-C4	6.39	1.38	1.34
33	BA	84	A	N3-C4	6.39	1.38	1.34
33	BA	574	A	N3-C4	6.39	1.38	1.34
33	BA	2007	A	N3-C4	6.39	1.38	1.34
1	AA	1260	A	N3-C4	6.39	1.38	1.34
33	BA	2835	A	N3-C4	6.39	1.38	1.34
1	AA	107	A	N3-C4	6.39	1.38	1.34
1	AA	1115	A	N3-C4	6.39	1.38	1.34
33	BA	947	A	N3-C4	6.39	1.38	1.34
33	BA	1569	A	N3-C4	6.39	1.38	1.34
1	AA	631	A	N3-C4	6.38	1.38	1.34
1	AA	862	A	N3-C4	6.38	1.38	1.34
1	AA	1247	A	N3-C4	6.38	1.38	1.34
33	BA	559	A	N3-C4	6.38	1.38	1.34
33	BA	1839	A	N3-C4	6.38	1.38	1.34
33	BA	1848	A	N3-C4	6.38	1.38	1.34
1	AA	271	A	N3-C4	6.38	1.38	1.34
1	AA	969	A	N3-C4	6.38	1.38	1.34
1	AA	1261	A	N3-C4	6.38	1.38	1.34
33	BA	198	A	N3-C4	6.38	1.38	1.34
33	BA	1724	A	N3-C4	6.38	1.38	1.34
1	AA	684	A	N3-C4	6.38	1.38	1.34
33	BA	1686	A	N3-C4	6.38	1.38	1.34
1	AA	381	A	N3-C4	6.38	1.38	1.34
1	AA	724	A	N3-C4	6.38	1.38	1.34
33	BA	342	A	N3-C4	6.38	1.38	1.34
33	BA	808	A	N3-C4	6.38	1.38	1.34
33	BA	829	A	N3-C4	6.38	1.38	1.34
33	BA	2389	A	N3-C4	6.38	1.38	1.34
1	AA	148	A	N3-C4	6.38	1.38	1.34
1	AA	1510	A	N3-C4	6.38	1.38	1.34
33	BA	65	A	N3-C4	6.38	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	279	A	N3-C4	6.38	1.38	1.34
33	BA	623	A	N3-C4	6.38	1.38	1.34
33	BA	2898	A	N3-C4	6.38	1.38	1.34
33	BA	993	A	N3-C4	6.38	1.38	1.34
1	AA	968	A	N3-C4	6.37	1.38	1.34
33	BA	821	A	N3-C4	6.37	1.38	1.34
33	BA	1179	A	N3-C4	6.37	1.38	1.34
33	BA	2052	A	N3-C4	6.37	1.38	1.34
33	BA	2547	A	N3-C4	6.37	1.38	1.34
33	BA	2618	A	N3-C4	6.37	1.38	1.34
1	AA	18	A	N3-C4	6.37	1.38	1.34
1	AA	206	A	N3-C4	6.37	1.38	1.34
1	AA	568	A	N3-C4	6.37	1.38	1.34
33	BA	630	A	N3-C4	6.37	1.38	1.34
33	BA	935	A	N3-C4	6.37	1.38	1.34
33	BA	1461	A	N3-C4	6.37	1.38	1.34
33	BA	2141	A	N3-C4	6.37	1.38	1.34
1	AA	211	A	N3-C4	6.37	1.38	1.34
33	BA	1047	A	N3-C4	6.37	1.38	1.34
33	BA	1697	A	N3-C4	6.37	1.38	1.34
33	BA	1802	A	N3-C4	6.37	1.38	1.34
33	BA	1918	A	N3-C4	6.37	1.38	1.34
1	AA	879	A	N3-C4	6.37	1.38	1.34
1	AA	1207	A	N3-C4	6.37	1.38	1.34
33	BA	337	A	N3-C4	6.37	1.38	1.34
33	BA	1265	A	N3-C4	6.37	1.38	1.34
33	BA	1734	A	N3-C4	6.37	1.38	1.34
33	BA	2616	A	N3-C4	6.37	1.38	1.34
33	BA	2807	A	N3-C4	6.37	1.38	1.34
1	AA	1133	A	N3-C4	6.36	1.38	1.34
1	AA	1188	A	N3-C4	6.36	1.38	1.34
33	BA	622	A	N3-C4	6.36	1.38	1.34
33	BA	2673	A	N3-C4	6.36	1.38	1.34
33	BA	2889	A	N3-C4	6.36	1.38	1.34
1	AA	329	A	N3-C4	6.36	1.38	1.34
1	AA	582	A	N3-C4	6.36	1.38	1.34
33	BA	849	A	N3-C4	6.36	1.38	1.34
1	AA	118	A	N3-C4	6.36	1.38	1.34
1	AA	236	A	N3-C4	6.36	1.38	1.34
1	AA	1443	A	N3-C4	6.36	1.38	1.34
1	AA	1528	A	N3-C4	6.36	1.38	1.34
33	BA	364	A	N3-C4	6.36	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	479	A	N3-C4	6.36	1.38	1.34
33	BA	1335	A	N3-C4	6.36	1.38	1.34
33	BA	1432	A	N3-C4	6.36	1.38	1.34
33	BA	71	A	N3-C4	6.36	1.38	1.34
1	AA	386	A	N3-C4	6.36	1.38	1.34
33	BA	2848	A	N3-C4	6.36	1.38	1.34
34	BB	25	A	N3-C4	6.36	1.38	1.34
1	AA	28	A	N3-C4	6.36	1.38	1.34
33	BA	389	A	N3-C4	6.36	1.38	1.34
33	BA	1648	A	N3-C4	6.36	1.38	1.34
33	BA	200	A	N3-C4	6.35	1.38	1.34
33	BA	965	A	N3-C4	6.35	1.38	1.34
33	BA	1026	A	N3-C4	6.35	1.38	1.34
33	BA	2454	A	N3-C4	6.35	1.38	1.34
1	AA	725	A	N3-C4	6.35	1.38	1.34
33	BA	162	A	N3-C4	6.35	1.38	1.34
33	BA	991	A	N3-C4	6.35	1.38	1.34
33	BA	2295	A	N3-C4	6.35	1.38	1.34
1	AA	581	A	N3-C4	6.35	1.38	1.34
33	BA	2398	A	N3-C4	6.35	1.38	1.34
33	BA	2498	A	N3-C4	6.35	1.38	1.34
33	BA	2132	A	N3-C4	6.35	1.38	1.34
34	BB	37	A	N3-C4	6.35	1.38	1.34
1	AA	690	A	N3-C4	6.35	1.38	1.34
33	BA	229	A	N3-C4	6.35	1.38	1.34
33	BA	496	A	N3-C4	6.35	1.38	1.34
33	BA	925	A	N3-C4	6.35	1.38	1.34
33	BA	2395	A	N3-C4	6.35	1.38	1.34
33	BA	2779	A	N3-C4	6.35	1.38	1.34
33	BA	717	A	N3-C4	6.34	1.38	1.34
33	BA	917	A	N3-C4	6.34	1.38	1.34
33	BA	2455	A	N3-C4	6.34	1.38	1.34
1	AA	984	A	N3-C4	6.34	1.38	1.34
33	BA	118	A	N3-C4	6.34	1.38	1.34
1	AA	1016	A	N3-C4	6.34	1.38	1.34
1	AA	1333	A	N3-C4	6.34	1.38	1.34
33	BA	2447	A	N3-C4	6.34	1.38	1.34
33	BA	354	A	N3-C4	6.34	1.38	1.34
33	BA	1078	A	N3-C4	6.34	1.38	1.34
33	BA	1722	A	N3-C4	6.34	1.38	1.34
33	BA	1850	A	N3-C4	6.34	1.38	1.34
1	AA	1407	A	N3-C4	6.33	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	170	A	N3-C4	6.33	1.38	1.34
33	BA	2296	A	N3-C4	6.33	1.38	1.34
1	AA	696	A	N3-C4	6.33	1.38	1.34
33	BA	1583	A	N3-C4	6.33	1.38	1.34
33	BA	1723	A	N3-C4	6.33	1.38	1.34
33	BA	1745	A	N3-C4	6.33	1.38	1.34
33	BA	1832	A	N3-C4	6.33	1.38	1.34
1	AA	929	A	N3-C4	6.33	1.38	1.34
33	BA	273	A	N3-C4	6.33	1.38	1.34
33	BA	1882	A	N3-C4	6.33	1.38	1.34
33	BA	2770	A	N3-C4	6.33	1.38	1.34
33	BA	220	A	N3-C4	6.33	1.38	1.34
33	BA	1982	A	N3-C4	6.33	1.38	1.34
1	AA	357	A	N3-C4	6.33	1.38	1.34
33	BA	2006	A	N3-C4	6.33	1.38	1.34
33	BA	2462	A	N3-C4	6.33	1.38	1.34
33	BA	216	A	N3-C4	6.33	1.38	1.34
33	BA	811	A	N3-C4	6.33	1.38	1.34
33	BA	1928	A	N3-C4	6.33	1.38	1.34
33	BA	2034	A	N3-C4	6.33	1.38	1.34
33	BA	2810	A	N3-C4	6.33	1.38	1.34
33	BA	2912	A	N3-C4	6.33	1.38	1.34
1	AA	604	A	N3-C4	6.32	1.38	1.34
33	BA	374	A	N3-C4	6.32	1.38	1.34
33	BA	830	A	N3-C4	6.32	1.38	1.34
33	BA	1947	A	N3-C4	6.32	1.38	1.34
1	AA	974	A	N3-C4	6.32	1.38	1.34
1	AA	1422	A	N3-C4	6.32	1.38	1.34
33	BA	957	A	N3-C4	6.32	1.38	1.34
33	BA	2302	A	N3-C4	6.32	1.38	1.34
1	AA	209	A	N3-C4	6.32	1.38	1.34
1	AA	743	A	N3-C4	6.32	1.38	1.34
33	BA	355	A	N3-C4	6.32	1.38	1.34
33	BA	673	A	N3-C4	6.32	1.38	1.34
33	BA	1291	A	N3-C4	6.32	1.38	1.34
1	AA	1112	A	N3-C4	6.32	1.38	1.34
33	BA	659	A	N3-C4	6.31	1.38	1.34
33	BA	2276	A	N3-C4	6.31	1.38	1.34
33	BA	2060	A	N3-C4	6.31	1.38	1.34
33	BA	746	A	N3-C4	6.31	1.38	1.34
33	BA	2062	A	N3-C4	6.31	1.38	1.34
33	BA	2606	A	N3-C4	6.31	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	582	A	N3-C4	6.31	1.38	1.34
33	BA	125	A	N3-C4	6.30	1.38	1.34
33	BA	1021	A	N3-C4	6.30	1.38	1.34
33	BA	1542	A	N3-C4	6.30	1.38	1.34
33	BA	1034	A	N3-C4	6.29	1.38	1.34
33	BA	1157	A	N3-C4	6.29	1.38	1.34
33	BA	1421	A	N3-C4	6.29	1.38	1.34
33	BA	2860	A	N3-C4	6.29	1.38	1.34
33	BA	2593	A	N3-C4	6.29	1.38	1.34
33	BA	2262	A	N3-C4	6.29	1.38	1.34
33	BA	2819	A	N3-C4	6.28	1.38	1.34
33	BA	2601	A	N3-C4	6.28	1.38	1.34
33	BA	2643	A	N3-C4	6.28	1.38	1.34
1	AA	1342	A	N3-C4	6.27	1.38	1.34
33	BA	179	A	N3-C4	6.27	1.38	1.34
33	BA	2026	A	N3-C4	6.27	1.38	1.34
33	BA	2357	A	N3-C4	6.27	1.38	1.34
1	AA	988	A	N3-C4	6.27	1.38	1.34
33	BA	178	A	N3-C4	6.26	1.38	1.34
33	BA	2477	A	N3-C4	6.26	1.38	1.34
1	AA	508	A	N3-C4	6.25	1.38	1.34
33	BA	2804	A	N3-C4	6.25	1.38	1.34
33	BA	1981	A	N3-C4	6.25	1.38	1.34
33	BA	1046	A	N3-C4	6.25	1.38	1.34
33	BA	1929	A	N3-C4	6.24	1.38	1.34
33	BA	1812	A	N3-C4	6.24	1.38	1.34
33	BA	1067	A	N3-C4	6.24	1.38	1.34
1	AA	583	A	N3-C4	6.23	1.38	1.34
1	AA	874	A	N3-C4	6.23	1.38	1.34
33	BA	2241	A	N3-C4	6.22	1.38	1.34
1	AA	555	A	N3-C4	6.22	1.38	1.34
33	BA	183	A	N3-C4	6.21	1.38	1.34
33	BA	2594	A	N3-C4	6.21	1.38	1.34
33	BA	1003	A	N3-C4	6.21	1.38	1.34
33	BA	67	A	N3-C4	6.20	1.38	1.34
33	BA	1074	A	N3-C4	6.20	1.38	1.34
33	BA	1201	A	N3-C4	6.19	1.38	1.34
1	AA	674	A	N3-C4	6.16	1.38	1.34
33	BA	490	A	N3-C4	6.16	1.38	1.34
33	BA	560	A	N3-C4	6.13	1.38	1.34
33	BA	667	A	N3-C4	6.12	1.38	1.34
33	BA	501	A	N3-C4	5.97	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AX	37	A	N7-C5	5.89	1.42	1.39
33	BA	1661	A	N7-C5	5.83	1.42	1.39
1	AA	1548	C	C2-N3	5.74	1.40	1.35
34	BB	99	A	C2-N3	5.40	1.38	1.33
1	AA	99	A	C2-N3	5.38	1.38	1.33
1	AA	507	A	C2-N3	5.34	1.38	1.33
1	AA	1026	A	C2-N3	5.33	1.38	1.33
33	BA	513	A	C2-N3	5.33	1.38	1.33
33	BA	1778	A	C2-N3	5.31	1.38	1.33
33	BA	1398	A	C2-N3	5.30	1.38	1.33
33	BA	2862	A	C2-N3	5.30	1.38	1.33
33	BA	1638	A	C2-N3	5.30	1.38	1.33
33	BA	1714	A	C2-N3	5.30	1.38	1.33
33	BA	527	A	C2-N3	5.29	1.38	1.33
1	AA	1166	A	C2-N3	5.28	1.38	1.33
33	BA	2436	A	C2-N3	5.26	1.38	1.33
33	BA	254	A	C2-N3	5.26	1.38	1.33
33	BA	910	A	C2-N3	5.26	1.38	1.33
33	BA	2735	A	C2-N3	5.26	1.38	1.33
33	BA	935	A	C2-N3	5.26	1.38	1.33
33	BA	2329	A	C2-N3	5.26	1.38	1.33
1	AA	405	A	C2-N3	5.25	1.38	1.33
33	BA	2844	A	C2-N3	5.25	1.38	1.33
33	BA	1103	A	C2-N3	5.25	1.38	1.33
1	AA	1160	A	C2-N3	5.24	1.38	1.33
33	BA	108	A	C2-N3	5.24	1.38	1.33
33	BA	736	A	C2-N3	5.24	1.38	1.33
33	BA	679	A	C2-N3	5.24	1.38	1.33
33	BA	2407	A	C2-N3	5.23	1.38	1.33
33	BA	56	A	C2-N3	5.23	1.38	1.33
33	BA	1286	A	C2-N3	5.23	1.38	1.33
33	BA	391	A	C2-N3	5.22	1.38	1.33
33	BA	2812	A	C2-N3	5.22	1.38	1.33
34	BB	46	A	C2-N3	5.22	1.38	1.33
33	BA	1006	A	C2-N3	5.21	1.38	1.33
33	BA	1816	A	C2-N3	5.21	1.38	1.33
1	AA	1278	A	C2-N3	5.21	1.38	1.33
33	BA	2663	A	C2-N3	5.21	1.38	1.33
1	AA	301	A	C2-N3	5.21	1.38	1.33
33	BA	1442	A	C2-N3	5.20	1.38	1.33
1	AA	933	A	C2-N3	5.20	1.38	1.33
1	AA	1272	A	C2-N3	5.20	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	649	A	C2-N3	5.20	1.38	1.33
33	BA	870	A	C2-N3	5.20	1.38	1.33
33	BA	1258	A	C2-N3	5.20	1.38	1.33
33	BA	1710	A	C2-N3	5.20	1.38	1.33
33	BA	2123	A	C2-N3	5.20	1.38	1.33
33	BA	2691	A	C2-N3	5.20	1.38	1.33
33	BA	1392	A	C2-N3	5.20	1.38	1.33
33	BA	2351	A	C2-N3	5.20	1.38	1.33
1	AA	844	A	C2-N3	5.19	1.38	1.33
1	AA	617	A	C2-N3	5.19	1.38	1.33
33	BA	1562	A	C2-N3	5.19	1.38	1.33
33	BA	2790	A	C2-N3	5.19	1.38	1.33
1	AA	1256	A	C2-N3	5.19	1.38	1.33
33	BA	722	A	C2-N3	5.19	1.38	1.33
33	BA	2164	A	C2-N3	5.19	1.38	1.33
33	BA	2627	A	C2-N3	5.19	1.38	1.33
1	AA	1384	A	C2-N3	5.19	1.38	1.33
33	BA	95	A	C2-N3	5.19	1.38	1.33
33	BA	2395	A	C2-N3	5.19	1.38	1.33
33	BA	185	A	C2-N3	5.18	1.38	1.33
33	BA	956	A	C2-N3	5.18	1.38	1.33
1	AA	74	A	C2-N3	5.18	1.38	1.33
21	AX	70	A	C2-N3	5.18	1.38	1.33
33	BA	1426	A	C2-N3	5.18	1.38	1.33
33	BA	656	A	C2-N3	5.18	1.38	1.33
33	BA	1709	A	C2-N3	5.18	1.38	1.33
33	BA	2500	A	C2-N3	5.18	1.38	1.33
33	BA	407	A	C2-N3	5.17	1.38	1.33
21	AX	24	A	C2-N3	5.17	1.38	1.33
1	AA	838	A	C2-N3	5.17	1.38	1.33
33	BA	634	A	C2-N3	5.17	1.38	1.33
33	BA	2831	A	C2-N3	5.17	1.38	1.33
1	AA	882	A	C2-N3	5.17	1.38	1.33
33	BA	90	A	C2-N3	5.17	1.38	1.33
34	BB	97	A	C2-N3	5.17	1.38	1.33
1	AA	948	A	C2-N3	5.17	1.38	1.33
1	AA	1022	A	C2-N3	5.17	1.38	1.33
33	BA	970	A	C2-N3	5.17	1.38	1.33
33	BA	2629	A	C2-N3	5.17	1.38	1.33
1	AA	391	A	C2-N3	5.16	1.38	1.33
1	AA	1427	A	C2-N3	5.16	1.38	1.33
1	AA	57	A	C2-N3	5.16	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	76	A	C2-N3	5.16	1.38	1.33
33	BA	156	A	C2-N3	5.16	1.38	1.33
33	BA	1667	A	C2-N3	5.16	1.38	1.33
33	BA	173	A	C2-N3	5.16	1.38	1.33
33	BA	1524	A	C2-N3	5.16	1.38	1.33
1	AA	1065	A	C2-N3	5.16	1.38	1.33
33	BA	2027	A	C2-N3	5.15	1.38	1.33
33	BA	517	A	C2-N3	5.15	1.38	1.33
33	BA	1126	A	C2-N3	5.15	1.38	1.33
33	BA	1675	A	C2-N3	5.15	1.38	1.33
33	BA	1858	A	C2-N3	5.15	1.38	1.33
33	BA	882	A	C2-N3	5.15	1.38	1.33
33	BA	2662	A	C2-N3	5.15	1.38	1.33
1	AA	605	A	C2-N3	5.15	1.38	1.33
33	BA	376	A	C2-N3	5.15	1.38	1.33
33	BA	2111	A	C2-N3	5.15	1.38	1.33
33	BA	1653	A	C2-N3	5.15	1.38	1.33
33	BA	1831	A	C2-N3	5.15	1.38	1.33
33	BA	2885	A	C2-N3	5.15	1.38	1.33
1	AA	282	A	C2-N3	5.14	1.38	1.33
1	AA	335	A	C2-N3	5.14	1.38	1.33
1	AA	721	A	C2-N3	5.14	1.38	1.33
1	AA	1349	A	C2-N3	5.14	1.38	1.33
33	BA	21	A	C2-N3	5.14	1.38	1.33
33	BA	715	A	C2-N3	5.14	1.38	1.33
33	BA	678	A	C2-N3	5.14	1.38	1.33
33	BA	1776	A	C2-N3	5.14	1.38	1.33
33	BA	2052	A	C2-N3	5.14	1.38	1.33
33	BA	2900	A	C2-N3	5.14	1.38	1.33
33	BA	518	A	C2-N3	5.13	1.38	1.33
33	BA	258	A	C2-N3	5.13	1.38	1.33
1	AA	337	A	C2-N3	5.13	1.38	1.33
33	BA	1618	A	C2-N3	5.13	1.38	1.33
33	BA	2270	A	C2-N3	5.13	1.38	1.33
1	AA	308	A	C2-N3	5.13	1.38	1.33
33	BA	630	A	C2-N3	5.13	1.38	1.33
1	AA	404	A	C2-N3	5.13	1.38	1.33
33	BA	41	A	C2-N3	5.13	1.38	1.33
33	BA	2078	A	C2-N3	5.13	1.38	1.33
33	BA	2163	A	C2-N3	5.12	1.38	1.33
1	AA	161	A	C2-N3	5.12	1.38	1.33
33	BA	673	A	C2-N3	5.12	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	974	A	C2-N3	5.12	1.38	1.33
33	BA	1096	A	C2-N3	5.12	1.38	1.33
33	BA	2106	A	C2-N3	5.12	1.38	1.33
1	AA	913	A	C2-N3	5.12	1.38	1.33
1	AA	1493	A	C2-N3	5.12	1.38	1.33
33	BA	2570	A	C2-N3	5.12	1.38	1.33
33	BA	1768	A	C2-N3	5.12	1.38	1.33
1	AA	1112	A	C2-N3	5.12	1.38	1.33
1	AA	1517	A	C2-N3	5.12	1.38	1.33
33	BA	538	A	C2-N3	5.12	1.38	1.33
33	BA	559	A	C2-N3	5.12	1.38	1.33
33	BA	769	A	C2-N3	5.12	1.38	1.33
33	BA	1100	A	C2-N3	5.12	1.38	1.33
33	BA	2754	A	C2-N3	5.12	1.38	1.33
33	BA	2846	A	C2-N3	5.12	1.38	1.33
33	BA	2893	A	C2-N3	5.12	1.38	1.33
1	AA	592	A	C2-N3	5.12	1.38	1.33
1	AA	34	A	C2-N3	5.12	1.38	1.33
1	AA	918	A	C2-N3	5.12	1.38	1.33
33	BA	724	A	C2-N3	5.12	1.38	1.33
33	BA	866	A	C2-N3	5.12	1.38	1.33
33	BA	1477	A	C2-N3	5.12	1.38	1.33
33	BA	1945	A	C2-N3	5.12	1.38	1.33
1	AA	604	A	C2-N3	5.11	1.38	1.33
33	BA	551	A	C2-N3	5.11	1.38	1.33
33	BA	786	A	C2-N3	5.11	1.38	1.33
33	BA	1895	A	C2-N3	5.11	1.38	1.33
33	BA	2205	A	C2-N3	5.11	1.38	1.33
33	BA	2722	A	C2-N3	5.11	1.38	1.33
33	BA	549	A	C2-N3	5.11	1.38	1.33
33	BA	1999	A	C2-N3	5.11	1.38	1.33
1	AA	548	A	C2-N3	5.11	1.38	1.33
1	AA	1490	A	C2-N3	5.11	1.38	1.33
33	BA	456	A	C2-N3	5.11	1.38	1.33
33	BA	1075	A	C2-N3	5.11	1.38	1.33
33	BA	1490	A	C2-N3	5.11	1.38	1.33
33	BA	307	A	C2-N3	5.11	1.38	1.33
34	BB	13	A	C2-N3	5.11	1.38	1.33
1	AA	433	A	C2-N3	5.11	1.38	1.33
1	AA	1425	A	C2-N3	5.11	1.38	1.33
33	BA	436	A	C2-N3	5.11	1.38	1.33
33	BA	1222	A	C2-N3	5.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1820	A	C2-N3	5.11	1.38	1.33
33	BA	2026	A	C2-N3	5.11	1.38	1.33
33	BA	318	A	C2-N3	5.10	1.38	1.33
33	BA	496	A	C2-N3	5.10	1.38	1.33
33	BA	1094	A	C2-N3	5.10	1.38	1.33
33	BA	2143	A	C2-N3	5.10	1.38	1.33
1	AA	512	A	C2-N3	5.10	1.38	1.33
1	AA	542	A	C2-N3	5.10	1.38	1.33
1	AA	996	A	C2-N3	5.10	1.38	1.33
33	BA	1839	A	C2-N3	5.10	1.38	1.33
33	BA	2381	A	C2-N3	5.10	1.38	1.33
33	BA	2511	A	C2-N3	5.10	1.38	1.33
33	BA	52	A	C2-N3	5.10	1.38	1.33
33	BA	130	A	C2-N3	5.10	1.38	1.33
33	BA	690	A	C2-N3	5.10	1.38	1.33
33	BA	1194	A	C2-N3	5.10	1.38	1.33
33	BA	1619	A	C2-N3	5.10	1.38	1.33
1	AA	278	A	C2-N3	5.10	1.38	1.33
1	AA	1188	A	C2-N3	5.10	1.38	1.33
33	BA	38	A	C2-N3	5.10	1.38	1.33
33	BA	1845	A	C2-N3	5.10	1.38	1.33
33	BA	2358	A	C2-N3	5.10	1.38	1.33
33	BA	2719	A	C2-N3	5.10	1.38	1.33
33	BA	2827	A	C2-N3	5.10	1.38	1.33
33	BA	2402	A	C2-N3	5.10	1.38	1.33
1	AA	234	A	C2-N3	5.09	1.38	1.33
1	AA	422	A	C2-N3	5.09	1.38	1.33
1	AA	1405	A	C2-N3	5.09	1.38	1.33
1	AA	1513	A	C2-N3	5.09	1.38	1.33
1	AA	1529	A	C2-N3	5.09	1.38	1.33
33	BA	889	A	C2-N3	5.09	1.38	1.33
33	BA	1791	A	C2-N3	5.09	1.38	1.33
33	BA	2369	A	C2-N3	5.09	1.38	1.33
33	BA	2668	A	C2-N3	5.09	1.38	1.33
33	BA	171	A	C2-N3	5.09	1.38	1.33
33	BA	1190	A	C2-N3	5.09	1.38	1.33
33	BA	1608	A	C2-N3	5.09	1.38	1.33
33	BA	913	A	C2-N3	5.09	1.38	1.33
33	BA	2498	A	C2-N3	5.09	1.38	1.33
1	AA	72	A	C2-N3	5.09	1.38	1.33
1	AA	984	A	C2-N3	5.09	1.38	1.33
1	AA	1115	A	C2-N3	5.09	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	144	A	C2-N3	5.09	1.38	1.33
33	BA	2389	A	C2-N3	5.09	1.38	1.33
1	AA	671	A	C2-N3	5.09	1.38	1.33
1	AA	1238	A	C2-N3	5.09	1.38	1.33
33	BA	236	A	C2-N3	5.09	1.38	1.33
33	BA	389	A	C2-N3	5.09	1.38	1.33
1	AA	271	A	C2-N3	5.09	1.38	1.33
1	AA	440	A	C2-N3	5.09	1.38	1.33
21	AX	9	A	C2-N3	5.09	1.38	1.33
33	BA	44	A	C2-N3	5.09	1.38	1.33
33	BA	326	A	C2-N3	5.09	1.38	1.33
33	BA	661	A	C2-N3	5.09	1.38	1.33
33	BA	830	A	C2-N3	5.09	1.38	1.33
33	BA	1025	A	C2-N3	5.09	1.38	1.33
33	BA	1424	A	C2-N3	5.09	1.38	1.33
1	AA	314	A	C2-N3	5.08	1.38	1.33
33	BA	168	A	C2-N3	5.08	1.38	1.33
33	BA	281	A	C2-N3	5.08	1.38	1.33
34	BB	43	A	C2-N3	5.08	1.38	1.33
1	AA	917	A	C2-N3	5.08	1.38	1.33
1	AA	956	A	C2-N3	5.08	1.38	1.33
1	AA	1161	A	C2-N3	5.08	1.38	1.33
33	BA	13	A	C2-N3	5.08	1.38	1.33
33	BA	462	A	C2-N3	5.08	1.38	1.33
33	BA	908	A	C2-N3	5.08	1.38	1.33
33	BA	1059	A	C2-N3	5.08	1.38	1.33
33	BA	1727	A	C2-N3	5.08	1.38	1.33
33	BA	1767	A	C2-N3	5.08	1.38	1.33
33	BA	2124	A	C2-N3	5.08	1.38	1.33
33	BA	2734	A	C2-N3	5.08	1.38	1.33
1	AA	67	A	C2-N3	5.08	1.38	1.33
1	AA	705	A	C2-N3	5.08	1.38	1.33
1	AA	911	A	C2-N3	5.08	1.38	1.33
1	AA	1437	A	C2-N3	5.08	1.38	1.33
21	AX	23	A	C2-N3	5.08	1.38	1.33
21	AX	76	A	C2-N3	5.08	1.38	1.33
33	BA	199	A	C2-N3	5.08	1.38	1.33
33	BA	1534	A	C2-N3	5.08	1.38	1.33
33	BA	2889	A	C2-N3	5.08	1.38	1.33
33	BA	2907	A	C2-N3	5.08	1.38	1.33
33	BA	2919	A	C2-N3	5.08	1.38	1.33
1	AA	1016	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	1270	A	C2-N3	5.08	1.38	1.33
33	BA	220	A	C2-N3	5.08	1.38	1.33
33	BA	2924	A	C2-N3	5.08	1.38	1.33
33	BA	260	A	C2-N3	5.08	1.38	1.33
33	BA	278	A	C2-N3	5.08	1.38	1.33
33	BA	616	A	C2-N3	5.08	1.38	1.33
33	BA	2302	A	C2-N3	5.08	1.38	1.33
33	BA	2904	A	C2-N3	5.08	1.38	1.33
1	AA	367	A	C2-N3	5.08	1.38	1.33
1	AA	1296	A	C2-N3	5.08	1.38	1.33
33	BA	1054	A	C2-N3	5.08	1.38	1.33
34	BB	27	A	C2-N3	5.08	1.38	1.33
1	AA	236	A	C2-N3	5.08	1.38	1.33
1	AA	715	A	C2-N3	5.08	1.38	1.33
1	AA	1417	A	C2-N3	5.08	1.38	1.33
33	BA	133	A	C2-N3	5.08	1.38	1.33
33	BA	763	A	C2-N3	5.08	1.38	1.33
33	BA	851	A	C2-N3	5.08	1.38	1.33
33	BA	1141	A	C2-N3	5.08	1.38	1.33
33	BA	1723	A	C2-N3	5.08	1.38	1.33
33	BA	2887	A	C2-N3	5.08	1.38	1.33
1	AA	875	A	C2-N3	5.07	1.38	1.33
1	AA	1236	A	C2-N3	5.07	1.38	1.33
1	AA	1327	A	C2-N3	5.07	1.38	1.33
33	BA	369	A	C2-N3	5.07	1.38	1.33
33	BA	1197	A	C2-N3	5.07	1.38	1.33
33	BA	1335	A	C2-N3	5.07	1.38	1.33
1	AA	685	A	C2-N3	5.07	1.38	1.33
33	BA	1357	A	C2-N3	5.07	1.38	1.33
33	BA	2923	A	C2-N3	5.07	1.38	1.33
1	AA	452	A	C2-N3	5.07	1.38	1.33
1	AA	968	A	C2-N3	5.07	1.38	1.33
1	AA	987	A	C2-N3	5.07	1.38	1.33
33	BA	193	A	C2-N3	5.07	1.38	1.33
33	BA	1947	A	C2-N3	5.07	1.38	1.33
33	BA	2117	A	C2-N3	5.07	1.38	1.33
1	AA	611	A	C2-N3	5.07	1.38	1.33
1	AA	727	A	C2-N3	5.07	1.38	1.33
33	BA	329	A	C2-N3	5.07	1.38	1.33
33	BA	1445	A	C2-N3	5.07	1.38	1.33
1	AA	140	A	C2-N3	5.07	1.38	1.33
1	AA	462	A	C2-N3	5.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	644	A	C2-N3	5.07	1.38	1.33
1	AA	1528	A	C2-N3	5.07	1.38	1.33
33	BA	828	A	C2-N3	5.07	1.38	1.33
33	BA	1734	A	C2-N3	5.07	1.38	1.33
33	BA	2421	A	C2-N3	5.07	1.38	1.33
1	AA	206	A	C2-N3	5.07	1.38	1.33
1	AA	371	A	C2-N3	5.07	1.38	1.33
1	AA	1143	A	C2-N3	5.07	1.38	1.33
1	AA	1435	A	C2-N3	5.07	1.38	1.33
33	BA	1235	A	C2-N3	5.07	1.38	1.33
33	BA	1788	A	C2-N3	5.07	1.38	1.33
33	BA	2100	A	C2-N3	5.07	1.38	1.33
33	BA	2220	A	C2-N3	5.07	1.38	1.33
33	BA	2256	A	C2-N3	5.07	1.38	1.33
33	BA	2455	A	C2-N3	5.07	1.38	1.33
34	BB	25	A	C2-N3	5.07	1.38	1.33
1	AA	352	A	C2-N3	5.06	1.38	1.33
1	AA	743	A	C2-N3	5.06	1.38	1.33
33	BA	964	A	C2-N3	5.06	1.38	1.33
33	BA	1393	A	C2-N3	5.06	1.38	1.33
1	AA	504	A	C2-N3	5.06	1.38	1.33
1	AA	768	A	C2-N3	5.06	1.38	1.33
33	BA	71	A	C2-N3	5.06	1.38	1.33
33	BA	1243	A	C2-N3	5.06	1.38	1.33
33	BA	1244	A	C2-N3	5.06	1.38	1.33
33	BA	2018	A	C2-N3	5.06	1.38	1.33
1	AA	225	A	C2-N3	5.06	1.38	1.33
1	AA	690	A	C2-N3	5.06	1.38	1.33
33	BA	230	A	C2-N3	5.06	1.38	1.33
33	BA	343	A	C2-N3	5.06	1.38	1.33
33	BA	429	A	C2-N3	5.06	1.38	1.33
33	BA	1406	A	C2-N3	5.06	1.38	1.33
34	BB	44	A	C2-N3	5.06	1.38	1.33
1	AA	485	A	C2-N3	5.06	1.38	1.33
1	AA	522	A	C2-N3	5.06	1.38	1.33
1	AA	638	A	C2-N3	5.06	1.38	1.33
1	AA	945	A	C2-N3	5.06	1.38	1.33
1	AA	1252	A	C2-N3	5.06	1.38	1.33
1	AA	1283	A	C2-N3	5.06	1.38	1.33
33	BA	790	A	C2-N3	5.06	1.38	1.33
33	BA	1008	A	C2-N3	5.06	1.38	1.33
33	BA	1260	A	C2-N3	5.06	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1627	A	C2-N3	5.06	1.38	1.33
33	BA	1636	A	C2-N3	5.06	1.38	1.33
33	BA	2406	A	C2-N3	5.06	1.38	1.33
33	BA	2826	A	C2-N3	5.06	1.38	1.33
1	AA	118	A	C2-N3	5.06	1.38	1.33
1	AA	650	A	C2-N3	5.06	1.38	1.33
1	AA	1102	A	C2-N3	5.06	1.38	1.33
1	AA	1369	A	C2-N3	5.06	1.38	1.33
33	BA	421	A	C2-N3	5.06	1.38	1.33
33	BA	507	A	C2-N3	5.06	1.38	1.33
33	BA	519	A	C2-N3	5.06	1.38	1.33
33	BA	1056	A	C2-N3	5.06	1.38	1.33
33	BA	1131	A	C2-N3	5.06	1.38	1.33
33	BA	1265	A	C2-N3	5.06	1.38	1.33
33	BA	2202	A	C2-N3	5.06	1.38	1.33
1	AA	658	A	C2-N3	5.06	1.38	1.33
33	BA	1797	A	C2-N3	5.06	1.38	1.33
33	BA	2134	A	C2-N3	5.06	1.38	1.33
33	BA	2170	A	C2-N3	5.06	1.38	1.33
1	AA	99	A	C5-C4	-5.05	1.35	1.38
1	AA	117	A	C2-N3	5.05	1.38	1.33
1	AA	142	A	C2-N3	5.05	1.38	1.33
1	AA	203	A	C2-N3	5.05	1.38	1.33
1	AA	507	A	C5-C4	-5.05	1.35	1.38
1	AA	823	A	C2-N3	5.05	1.38	1.33
1	AA	919	A	C2-N3	5.05	1.38	1.33
1	AA	1503	A	C2-N3	5.05	1.38	1.33
21	AX	44	A	C2-N3	5.05	1.38	1.33
33	BA	305	A	C2-N3	5.05	1.38	1.33
33	BA	758	A	C2-N3	5.05	1.38	1.33
33	BA	1019	A	C2-N3	5.05	1.38	1.33
33	BA	1179	A	C2-N3	5.05	1.38	1.33
33	BA	1284	A	C2-N3	5.05	1.38	1.33
33	BA	1316	A	C2-N3	5.05	1.38	1.33
33	BA	1347	A	C2-N3	5.05	1.38	1.33
33	BA	1966	A	C2-N3	5.05	1.38	1.33
33	BA	2837	A	C2-N3	5.05	1.38	1.33
33	BA	677	A	C2-N3	5.05	1.38	1.33
33	BA	1541	A	C2-N3	5.05	1.38	1.33
33	BA	1606	A	C2-N3	5.05	1.38	1.33
33	BA	1655	A	C2-N3	5.05	1.38	1.33
1	AA	160	A	C2-N3	5.05	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	296	A	C2-N3	5.05	1.38	1.33
1	AA	758	A	C2-N3	5.05	1.38	1.33
1	AA	793	A	C2-N3	5.05	1.38	1.33
1	AA	883	A	C2-N3	5.05	1.38	1.33
33	BA	428	A	C2-N3	5.05	1.38	1.33
33	BA	1254	A	C2-N3	5.05	1.38	1.33
33	BA	1989	A	C2-N3	5.05	1.38	1.33
33	BA	1998	A	C2-N3	5.05	1.38	1.33
1	AA	679	A	C2-N3	5.05	1.38	1.33
1	AA	1028	A	C2-N3	5.05	1.38	1.33
1	AA	1111	A	C2-N3	5.05	1.38	1.33
33	BA	692	A	C2-N3	5.05	1.38	1.33
33	BA	1221	A	C2-N3	5.05	1.38	1.33
33	BA	2119	A	C2-N3	5.05	1.38	1.33
33	BA	2176	A	C2-N3	5.05	1.38	1.33
34	BB	56	A	C2-N3	5.05	1.38	1.33
1	AA	724	A	C2-N3	5.05	1.38	1.33
1	AA	1510	A	C2-N3	5.05	1.38	1.33
21	AX	21	A	C2-N3	5.05	1.38	1.33
33	BA	1277	A	C2-N3	5.05	1.38	1.33
33	BA	1888	A	C2-N3	5.05	1.38	1.33
33	BA	2769	A	C2-N3	5.05	1.38	1.33
1	AA	210	A	C2-N3	5.05	1.38	1.33
1	AA	364	A	C2-N3	5.05	1.38	1.33
1	AA	664	A	C2-N3	5.05	1.38	1.33
1	AA	824	A	C2-N3	5.05	1.38	1.33
1	AA	902	A	C2-N3	5.05	1.38	1.33
1	AA	928	A	C2-N3	5.05	1.38	1.33
1	AA	1315	A	C2-N3	5.05	1.38	1.33
33	BA	268	A	C2-N3	5.05	1.38	1.33
33	BA	543	A	C2-N3	5.05	1.38	1.33
33	BA	1224	A	C2-N3	5.05	1.38	1.33
33	BA	1499	A	C2-N3	5.05	1.38	1.33
1	AA	381	A	C2-N3	5.04	1.38	1.33
1	AA	1206	A	C2-N3	5.04	1.38	1.33
1	AA	1320	A	C2-N3	5.04	1.38	1.33
33	BA	314	A	C2-N3	5.04	1.38	1.33
33	BA	2459	A	C2-N3	5.04	1.38	1.33
1	AA	796	A	C2-N3	5.04	1.38	1.33
1	AA	1434	A	C2-N3	5.04	1.38	1.33
33	BA	486	A	C2-N3	5.04	1.38	1.33
33	BA	547	A	C2-N3	5.04	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	876	A	C2-N3	5.04	1.38	1.33
33	BA	917	A	C2-N3	5.04	1.38	1.33
33	BA	1142	A	C2-N3	5.04	1.38	1.33
33	BA	1314	A	C2-N3	5.04	1.38	1.33
33	BA	1700	A	C2-N3	5.04	1.38	1.33
33	BA	1743	A	C2-N3	5.04	1.38	1.33
33	BA	2043	A	C2-N3	5.04	1.38	1.33
33	BA	2044	A	C2-N3	5.04	1.38	1.33
33	BA	2047	A	C2-N3	5.04	1.38	1.33
1	AA	35	A	C2-N3	5.04	1.38	1.33
1	AA	659	A	C2-N3	5.04	1.38	1.33
1	AA	947	A	C2-N3	5.04	1.38	1.33
1	AA	1140	A	C2-N3	5.04	1.38	1.33
1	AA	1478	A	C2-N3	5.04	1.38	1.33
33	BA	117	A	C2-N3	5.04	1.38	1.33
33	BA	1034	A	C2-N3	5.04	1.38	1.33
33	BA	1981	A	C2-N3	5.04	1.38	1.33
33	BA	2441	A	C2-N3	5.04	1.38	1.33
33	BA	2779	A	C2-N3	5.04	1.38	1.33
1	AA	1248	A	C2-N3	5.04	1.38	1.33
33	BA	500	A	C2-N3	5.04	1.38	1.33
33	BA	762	A	C2-N3	5.04	1.38	1.33
33	BA	1483	A	C2-N3	5.04	1.38	1.33
33	BA	1672	A	C2-N3	5.04	1.38	1.33
33	BA	1802	A	C2-N3	5.04	1.38	1.33
33	BA	2200	A	C2-N3	5.04	1.38	1.33
33	BA	2227	A	C2-N3	5.04	1.38	1.33
33	BA	2252	A	C2-N3	5.04	1.38	1.33
34	BB	37	A	C2-N3	5.04	1.38	1.33
1	AA	228	A	C2-N3	5.04	1.38	1.33
1	AA	1189	A	C2-N3	5.04	1.38	1.33
1	AA	1442	A	C2-N3	5.04	1.38	1.33
1	AA	1470	A	C2-N3	5.04	1.38	1.33
33	BA	752	A	C2-N3	5.04	1.38	1.33
33	BA	1026	A	C2-N3	5.04	1.38	1.33
33	BA	1233	A	C2-N3	5.04	1.38	1.33
33	BA	1695	A	C2-N3	5.04	1.38	1.33
33	BA	1901	A	C2-N3	5.04	1.38	1.33
33	BA	2349	A	C2-N3	5.04	1.38	1.33
1	AA	979	A	C2-N3	5.04	1.38	1.33
33	BA	469	A	C2-N3	5.04	1.38	1.33
33	BA	1533	A	C2-N3	5.04	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1583	A	C2-N3	5.04	1.38	1.33
33	BA	1900	A	C2-N3	5.04	1.38	1.33
33	BA	2030	A	C2-N3	5.04	1.38	1.33
34	BB	51	A	C2-N3	5.04	1.38	1.33
1	AA	55	A	C2-N3	5.04	1.38	1.33
1	AA	786	A	C2-N3	5.04	1.38	1.33
1	AA	1179	A	C2-N3	5.04	1.38	1.33
33	BA	5	A	C2-N3	5.04	1.38	1.33
33	BA	705	A	C2-N3	5.04	1.38	1.33
33	BA	1617	A	C2-N3	5.04	1.38	1.33
33	BA	1746	A	C2-N3	5.04	1.38	1.33
33	BA	2590	A	C2-N3	5.04	1.38	1.33
33	BA	2616	A	C2-N3	5.04	1.38	1.33
33	BA	2619	A	C2-N3	5.04	1.38	1.33
33	BA	2805	A	C2-N3	5.04	1.38	1.33
1	AA	281	A	C2-N3	5.03	1.38	1.33
1	AA	397	A	C2-N3	5.03	1.38	1.33
1	AA	777	A	C2-N3	5.03	1.38	1.33
33	BA	6	A	C2-N3	5.03	1.38	1.33
33	BA	150	A	C2-N3	5.03	1.38	1.33
33	BA	740	A	C2-N3	5.03	1.38	1.33
33	BA	1588	A	C2-N3	5.03	1.38	1.33
33	BA	2447	A	C2-N3	5.03	1.38	1.33
34	BB	39	A	C2-N3	5.03	1.38	1.33
1	AA	491	A	C2-N3	5.03	1.38	1.33
1	AA	1257	A	C2-N3	5.03	1.38	1.33
33	BA	49	A	C2-N3	5.03	1.38	1.33
33	BA	431	A	C2-N3	5.03	1.38	1.33
33	BA	1615	A	C2-N3	5.03	1.38	1.33
33	BA	2141	A	C2-N3	5.03	1.38	1.33
1	AA	173	A	C2-N3	5.03	1.38	1.33
1	AA	287	A	C2-N3	5.03	1.38	1.33
1	AA	730	A	C2-N3	5.03	1.38	1.33
1	AA	1178	A	C2-N3	5.03	1.38	1.33
1	AA	1180	A	C2-N3	5.03	1.38	1.33
1	AA	1271	A	C2-N3	5.03	1.38	1.33
21	AX	41	A	C2-N3	5.03	1.38	1.33
33	BA	275	A	C2-N3	5.03	1.38	1.33
33	BA	1877	A	C2-N3	5.03	1.38	1.33
33	BA	1885	A	C2-N3	5.03	1.38	1.33
33	BA	1906	A	C2-N3	5.03	1.38	1.33
33	BA	2216	A	C2-N3	5.03	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2593	A	C2-N3	5.03	1.38	1.33
1	AA	290	A	C2-N3	5.03	1.38	1.33
1	AA	910	A	C2-N3	5.03	1.38	1.33
1	AA	1463	A	C2-N3	5.03	1.38	1.33
33	BA	1134	A	C2-N3	5.03	1.38	1.33
1	AA	114	A	C2-N3	5.03	1.38	1.33
1	AA	306	A	C2-N3	5.03	1.38	1.33
1	AA	1342	A	C2-N3	5.03	1.38	1.33
33	BA	1020	A	C2-N3	5.03	1.38	1.33
33	BA	1542	A	C2-N3	5.03	1.38	1.33
33	BA	1593	A	C2-N3	5.03	1.38	1.33
33	BA	1928	A	C2-N3	5.03	1.38	1.33
33	BA	1929	A	C2-N3	5.03	1.38	1.33
33	BA	2526	A	C2-N3	5.03	1.38	1.33
33	BA	2787	A	C2-N3	5.03	1.38	1.33
1	AA	139	A	C2-N3	5.03	1.38	1.33
1	AA	423	A	C2-N3	5.03	1.38	1.33
1	AA	1245	A	C2-N3	5.03	1.38	1.33
1	AA	1297	A	C2-N3	5.03	1.38	1.33
33	BA	868	A	C2-N3	5.03	1.38	1.33
33	BA	1480	A	C2-N3	5.03	1.38	1.33
33	BA	1677	A	C2-N3	5.03	1.38	1.33
33	BA	2356	A	C2-N3	5.03	1.38	1.33
33	BA	2875	A	C2-N3	5.03	1.38	1.33
33	BA	14	A	C2-N3	5.02	1.38	1.33
33	BA	198	A	C2-N3	5.02	1.38	1.33
33	BA	388	A	C2-N3	5.02	1.38	1.33
33	BA	896	A	C2-N3	5.02	1.38	1.33
33	BA	1485	A	C2-N3	5.02	1.38	1.33
33	BA	1620	A	C2-N3	5.02	1.38	1.33
33	BA	1686	A	C2-N3	5.02	1.38	1.33
33	BA	2307	A	C2-N3	5.02	1.38	1.33
33	BA	2343	A	C2-N3	5.02	1.38	1.33
1	AA	357	A	C2-N3	5.02	1.38	1.33
1	AA	541	A	C2-N3	5.02	1.38	1.33
1	AA	669	A	C2-N3	5.02	1.38	1.33
1	AA	1155	A	C2-N3	5.02	1.38	1.33
33	BA	337	A	C2-N3	5.02	1.38	1.33
33	BA	947	A	C2-N3	5.02	1.38	1.33
33	BA	1504	A	C2-N3	5.02	1.38	1.33
33	BA	1517	A	C2-N3	5.02	1.38	1.33
33	BA	1585	A	C2-N3	5.02	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1722	A	C2-N3	5.02	1.38	1.33
33	BA	2071	A	C2-N3	5.02	1.38	1.33
33	BA	2298	A	C2-N3	5.02	1.38	1.33
33	BA	2480	A	C2-N3	5.02	1.38	1.33
33	BA	2673	A	C2-N3	5.02	1.38	1.33
34	BB	17	A	C2-N3	5.02	1.38	1.33
34	BB	50	A	C2-N3	5.02	1.38	1.33
1	AA	870	A	C2-N3	5.02	1.38	1.33
33	BA	943	A	C2-N3	5.02	1.38	1.33
33	BA	2000	A	C2-N3	5.02	1.38	1.33
1	AA	266	A	C2-N3	5.02	1.38	1.33
1	AA	439	A	C2-N3	5.02	1.38	1.33
1	AA	1056	A	C2-N3	5.02	1.38	1.33
1	AA	1092	A	C2-N3	5.02	1.38	1.33
1	AA	1200	A	C2-N3	5.02	1.38	1.33
33	BA	699	A	C2-N3	5.02	1.38	1.33
33	BA	1005	A	C2-N3	5.02	1.38	1.33
33	BA	1113	A	C2-N3	5.02	1.38	1.33
33	BA	1144	A	C2-N3	5.02	1.38	1.33
33	BA	1942	A	C2-N3	5.02	1.38	1.33
33	BA	2497	A	C2-N3	5.02	1.38	1.33
33	BA	2794	A	C2-N3	5.02	1.38	1.33
1	AA	81	A	C2-N3	5.02	1.38	1.33
1	AA	438	A	C2-N3	5.02	1.38	1.33
1	AA	460	A	C2-N3	5.02	1.38	1.33
1	AA	1103	A	C2-N3	5.02	1.38	1.33
1	AA	1451	A	C2-N3	5.02	1.38	1.33
33	BA	225	A	C2-N3	5.02	1.38	1.33
33	BA	229	A	C2-N3	5.02	1.38	1.33
33	BA	259	A	C2-N3	5.02	1.38	1.33
33	BA	475	A	C2-N3	5.02	1.38	1.33
33	BA	753	A	C2-N3	5.02	1.38	1.33
33	BA	782	A	C2-N3	5.02	1.38	1.33
33	BA	1042	A	C2-N3	5.02	1.38	1.33
33	BA	1569	A	C2-N3	5.02	1.38	1.33
1	AA	811	A	C2-N3	5.02	1.38	1.33
33	BA	537	A	C2-N3	5.02	1.38	1.33
33	BA	1461	A	C2-N3	5.02	1.38	1.33
33	BA	1520	A	C2-N3	5.02	1.38	1.33
1	AA	684	A	C2-N3	5.01	1.38	1.33
1	AA	1366	A	C2-N3	5.01	1.38	1.33
33	BA	1464	A	C2-N3	5.01	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	1882	A	C2-N3	5.01	1.38	1.33
33	BA	1914	A	C2-N3	5.01	1.38	1.33
33	BA	2148	A	C2-N3	5.01	1.38	1.33
33	BA	2387	A	C2-N3	5.01	1.38	1.33
33	BA	2704	A	C2-N3	5.01	1.38	1.33
1	AA	501	A	C2-N3	5.01	1.38	1.33
1	AA	618	A	C2-N3	5.01	1.38	1.33
33	BA	364	A	C2-N3	5.01	1.38	1.33
33	BA	530	A	C2-N3	5.01	1.38	1.33
33	BA	1084	A	C2-N3	5.01	1.38	1.33
33	BA	1174	A	C2-N3	5.01	1.38	1.33
33	BA	1850	A	C2-N3	5.01	1.38	1.33
1	AA	211	A	C2-N3	5.01	1.38	1.33
1	AA	390	A	C2-N3	5.01	1.38	1.33
1	AA	1455	A	C2-N3	5.01	1.38	1.33
33	BA	102	A	C2-N3	5.01	1.38	1.33
33	BA	971	A	C2-N3	5.01	1.38	1.33
33	BA	1575	A	C2-N3	5.01	1.38	1.33
1	AA	568	A	C2-N3	5.01	1.38	1.33
1	AA	677	A	C2-N3	5.01	1.38	1.33
1	AA	790	A	C2-N3	5.01	1.38	1.33
1	AA	1266	A	C2-N3	5.01	1.38	1.33
33	BA	166	A	C2-N3	5.01	1.38	1.33
33	BA	265	A	C2-N3	5.01	1.38	1.33
33	BA	339	A	C2-N3	5.01	1.38	1.33
33	BA	476	A	C2-N3	5.01	1.38	1.33
33	BA	637	A	C2-N3	5.01	1.38	1.33
33	BA	1014	A	C2-N3	5.01	1.38	1.33
33	BA	1313	A	C2-N3	5.01	1.38	1.33
33	BA	1491	A	C2-N3	5.01	1.38	1.33
33	BA	1601	A	C2-N3	5.01	1.38	1.33
33	BA	2049	A	C2-N3	5.01	1.38	1.33
33	BA	2462	A	C2-N3	5.01	1.38	1.33
33	BA	2750	A	C2-N3	5.01	1.38	1.33
1	AA	651	A	C2-N3	5.01	1.38	1.33
1	AA	1213	A	C2-N3	5.01	1.38	1.33
1	AA	1261	A	C2-N3	5.01	1.38	1.33
33	BA	991	A	C2-N3	5.01	1.38	1.33
33	BA	1029	A	C2-N3	5.01	1.38	1.33
33	BA	1066	A	C2-N3	5.01	1.38	1.33
33	BA	2152	A	C2-N3	5.01	1.38	1.33
33	BA	2417	A	C2-N3	5.01	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2507	A	C2-N3	5.01	1.38	1.33
33	BA	2594	A	C2-N3	5.01	1.38	1.33
33	BA	2807	A	C2-N3	5.01	1.38	1.33
1	AA	10	A	C2-N3	5.01	1.38	1.33
1	AA	94	A	C2-N3	5.01	1.38	1.33
1	AA	254	A	C2-N3	5.01	1.38	1.33
1	AA	496	A	C2-N3	5.01	1.38	1.33
1	AA	1014	A	C2-N3	5.01	1.38	1.33
1	AA	1048	A	C2-N3	5.01	1.38	1.33
33	BA	553	A	C2-N3	5.01	1.38	1.33
33	BA	1506	A	C2-N3	5.01	1.38	1.33
33	BA	1848	A	C2-N3	5.01	1.38	1.33
33	BA	2317	A	C2-N3	5.01	1.38	1.33
33	BA	2463	A	C2-N3	5.01	1.38	1.33
33	BA	2517	A	C2-N3	5.01	1.38	1.33
33	BA	2532	A	C2-N3	5.01	1.38	1.33
33	BA	2661	A	C2-N3	5.01	1.38	1.33
33	BA	2762	A	C2-N3	5.01	1.38	1.33
1	AA	1294	A	C2-N3	5.00	1.38	1.33
33	BA	384	A	C2-N3	5.00	1.38	1.33
1	AA	240	A	C2-N3	5.00	1.38	1.33
1	AA	518	A	C2-N3	5.00	1.38	1.33
1	AA	1328	A	C2-N3	5.00	1.38	1.33
1	AA	1383	A	C2-N3	5.00	1.38	1.33
33	BA	124	A	C2-N3	5.00	1.38	1.33
33	BA	325	A	C2-N3	5.00	1.38	1.33
33	BA	548	A	C2-N3	5.00	1.38	1.33
33	BA	1119	A	C2-N3	5.00	1.38	1.33
33	BA	1721	A	C2-N3	5.00	1.38	1.33
33	BA	1815	A	C2-N3	5.00	1.38	1.33
34	BB	18	A	C2-N3	5.00	1.38	1.33
34	BB	20	A	C2-N3	5.00	1.38	1.33
1	AA	382	A	C2-N3	5.00	1.38	1.33
1	AA	725	A	C2-N3	5.00	1.38	1.33
1	AA	738	A	C2-N3	5.00	1.38	1.33
1	AA	757	A	C2-N3	5.00	1.38	1.33
1	AA	1205	A	C2-N3	5.00	1.38	1.33
33	BA	53	A	C2-N3	5.00	1.38	1.33
33	BA	727	A	C2-N3	5.00	1.38	1.33
33	BA	1027	A	C2-N3	5.00	1.38	1.33
33	BA	1326	A	C2-N3	5.00	1.38	1.33
33	BA	2146	A	C2-N3	5.00	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BA	2303	A	C2-N3	5.00	1.38	1.33
33	BA	2658	A	C2-N3	5.00	1.38	1.33

All (11797) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1134	A	C2-N3-C4	20.56	120.88	110.60
33	BA	226	A	C2-N3-C4	20.47	120.84	110.60
33	BA	1691	A	C2-N3-C4	20.46	120.83	110.60
1	AA	1308	A	C2-N3-C4	20.36	120.78	110.60
1	AA	195	A	C2-N3-C4	20.24	120.72	110.60
1	AA	993	A	C2-N3-C4	20.15	120.68	110.60
33	BA	732	A	C2-N3-C4	20.15	120.67	110.60
33	BA	593	A	C2-N3-C4	20.02	120.61	110.60
33	BA	1581	A	C2-N3-C4	20.01	120.61	110.60
1	AA	405	A	C2-N3-C4	19.89	120.54	110.60
33	BA	1714	A	C2-N3-C4	19.88	120.54	110.60
1	AA	572	A	C2-N3-C4	19.79	120.49	110.60
1	AA	1234	A	C2-N3-C4	19.78	120.49	110.60
33	BA	1046	A	C2-N3-C4	19.71	120.45	110.60
1	AA	1288	A	C2-N3-C4	19.67	120.44	110.60
33	BA	560	A	C2-N3-C4	19.60	120.40	110.60
1	AA	674	A	C2-N3-C4	19.53	120.37	110.60
33	BA	913	A	C2-N3-C4	19.52	120.36	110.60
1	AA	987	A	C2-N3-C4	19.50	120.35	110.60
33	BA	1491	A	C2-N3-C4	19.48	120.34	110.60
33	BA	2786	A	C2-N3-C4	19.47	120.34	110.60
33	BA	1506	A	C2-N3-C4	19.45	120.33	110.60
33	BA	438	A	C2-N3-C4	19.44	120.32	110.60
33	BA	925	A	C2-N3-C4	19.42	120.31	110.60
33	BA	1480	A	C2-N3-C4	19.42	120.31	110.60
33	BA	1132	A	C2-N3-C4	19.41	120.31	110.60
33	BA	948	A	C2-N3-C4	19.41	120.31	110.60
34	BB	11	A	C2-N3-C4	19.40	120.30	110.60
33	BA	1073	A	C2-N3-C4	19.40	120.30	110.60
33	BA	1360	A	C2-N3-C4	19.37	120.29	110.60
33	BA	2532	A	C2-N3-C4	19.37	120.29	110.60
33	BA	765	A	C2-N3-C4	19.36	120.28	110.60
1	AA	507	A	C2-N3-C4	19.36	120.28	110.60
33	BA	2202	A	C2-N3-C4	19.35	120.28	110.60
33	BA	527	A	C2-N3-C4	19.35	120.27	110.60
33	BA	935	A	C2-N3-C4	19.35	120.27	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	732	A	N1-C2-N3	-19.34	119.63	129.30
33	BA	437	A	C2-N3-C4	19.33	120.27	110.60
1	AA	1341	A	C2-N3-C4	19.33	120.27	110.60
33	BA	2339	A	C2-N3-C4	19.33	120.26	110.60
33	BA	2794	A	C2-N3-C4	19.32	120.26	110.60
33	BA	390	A	C2-N3-C4	19.32	120.26	110.60
33	BA	2143	A	C2-N3-C4	19.32	120.26	110.60
1	AA	128	A	C2-N3-C4	19.30	120.25	110.60
1	AA	727	A	C2-N3-C4	19.30	120.25	110.60
33	BA	957	A	C2-N3-C4	19.29	120.24	110.60
1	AA	631	A	N1-C2-N3	-19.28	119.66	129.30
33	BA	1905	A	C2-N3-C4	19.27	120.24	110.60
1	AA	1372	A	N1-C2-N3	-19.26	119.67	129.30
33	BA	1562	A	C2-N3-C4	19.26	120.23	110.60
33	BA	1667	A	C2-N3-C4	19.25	120.22	110.60
33	BA	849	A	C2-N3-C4	19.25	120.22	110.60
1	AA	1358	A	C2-N3-C4	19.22	120.21	110.60
33	BA	574	A	C2-N3-C4	19.21	120.21	110.60
33	BA	1555	A	N1-C2-N3	-19.20	119.70	129.30
33	BA	1536	A	C2-N3-C4	19.20	120.20	110.60
33	BA	353	A	C2-N3-C4	19.19	120.20	110.60
1	AA	674	A	N1-C2-N3	-19.19	119.70	129.30
1	AA	508	A	N1-C2-N3	-19.19	119.71	129.30
1	AA	630	A	C2-N3-C4	19.19	120.19	110.60
33	BA	1019	A	C2-N3-C4	19.19	120.19	110.60
34	BB	71	A	C2-N3-C4	19.19	120.19	110.60
1	AA	1358	A	N1-C2-N3	-19.19	119.71	129.30
33	BA	736	A	C2-N3-C4	19.19	120.19	110.60
1	AA	555	A	C2-N3-C4	19.18	120.19	110.60
33	BA	1005	A	C2-N3-C4	19.18	120.19	110.60
33	BA	2689	A	C2-N3-C4	19.18	120.19	110.60
1	AA	1178	A	C2-N3-C4	19.18	120.19	110.60
33	BA	1305	A	N1-C2-N3	-19.17	119.72	129.30
1	AA	956	A	C2-N3-C4	19.17	120.18	110.60
33	BA	1029	A	C2-N3-C4	19.16	120.18	110.60
33	BA	1877	A	C2-N3-C4	19.15	120.18	110.60
1	AA	1143	A	C2-N3-C4	19.14	120.17	110.60
33	BA	1905	A	N1-C2-N3	-19.14	119.73	129.30
1	AA	862	A	N1-C2-N3	-19.14	119.73	129.30
33	BA	1123	A	N1-C2-N3	-19.14	119.73	129.30
33	BA	1074	A	C2-N3-C4	19.13	120.17	110.60
33	BA	1157	A	C2-N3-C4	19.13	120.17	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	737	A	C2-N3-C4	19.13	120.17	110.60
33	BA	2049	A	C2-N3-C4	19.13	120.17	110.60
33	BA	183	A	N1-C2-N3	-19.13	119.74	129.30
1	AA	151	A	C2-N3-C4	19.12	120.16	110.60
33	BA	2848	A	C2-N3-C4	19.12	120.16	110.60
33	BA	1930	A	C2-N3-C4	19.11	120.15	110.60
21	AX	23	A	C2-N3-C4	19.10	120.15	110.60
33	BA	2547	A	C2-N3-C4	19.10	120.15	110.60
33	BA	1485	A	C2-N3-C4	19.10	120.15	110.60
33	BA	2735	A	C2-N3-C4	19.09	120.15	110.60
33	BA	689	A	C2-N3-C4	19.09	120.15	110.60
33	BA	2062	A	N1-C2-N3	-19.09	119.75	129.30
33	BA	1900	A	C2-N3-C4	19.09	120.15	110.60
1	AA	631	A	C2-N3-C4	19.09	120.14	110.60
1	AA	1155	A	C2-N3-C4	19.09	120.14	110.60
1	AA	114	A	C2-N3-C4	19.09	120.14	110.60
33	BA	526	A	N1-C2-N3	-19.09	119.76	129.30
33	BA	2459	A	C2-N3-C4	19.09	120.14	110.60
1	AA	1160	A	C2-N3-C4	19.08	120.14	110.60
1	AA	844	A	C2-N3-C4	19.08	120.14	110.60
33	BA	1473	A	N1-C2-N3	-19.07	119.77	129.30
1	AA	457	A	C2-N3-C4	19.07	120.13	110.60
1	AA	477	A	C2-N3-C4	19.07	120.13	110.60
33	BA	526	A	C2-N3-C4	19.07	120.13	110.60
33	BA	943	A	C2-N3-C4	19.07	120.14	110.60
1	AA	1260	A	C2-N3-C4	19.07	120.13	110.60
21	AX	14	A	C2-N3-C4	19.07	120.13	110.60
1	AA	1004	A	C2-N3-C4	19.06	120.13	110.60
33	BA	765	A	N1-C2-N3	-19.06	119.77	129.30
33	BA	185	A	C2-N3-C4	19.06	120.13	110.60
34	BB	13	A	C2-N3-C4	19.06	120.13	110.60
1	AA	282	A	C2-N3-C4	19.06	120.13	110.60
33	BA	1417	A	N1-C2-N3	-19.06	119.77	129.30
1	AA	151	A	N1-C2-N3	-19.06	119.77	129.30
33	BA	1398	A	C2-N3-C4	19.05	120.13	110.60
33	BA	2083	A	C2-N3-C4	19.05	120.13	110.60
33	BA	1388	A	C2-N3-C4	19.05	120.13	110.60
33	BA	2826	A	C2-N3-C4	19.05	120.13	110.60
33	BA	1286	A	C2-N3-C4	19.05	120.12	110.60
1	AA	150	A	N1-C2-N3	-19.05	119.78	129.30
33	BA	2351	A	C2-N3-C4	19.05	120.12	110.60
33	BA	133	A	C2-N3-C4	19.05	120.12	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	504	A	N1-C2-N3	-19.05	119.78	129.30
33	BA	2329	A	C2-N3-C4	19.05	120.12	110.60
33	BA	281	A	C2-N3-C4	19.04	120.12	110.60
33	BA	1524	A	C2-N3-C4	19.04	120.12	110.60
33	BA	108	A	C2-N3-C4	19.04	120.12	110.60
33	BA	2807	A	N1-C2-N3	-19.04	119.78	129.30
1	AA	170	A	C2-N3-C4	19.04	120.12	110.60
33	BA	715	A	C2-N3-C4	19.03	120.12	110.60
33	BA	1097	A	C2-N3-C4	19.03	120.12	110.60
33	BA	1421	A	C2-N3-C4	19.03	120.12	110.60
33	BA	1885	A	C2-N3-C4	19.03	120.12	110.60
1	AA	439	A	C2-N3-C4	19.03	120.11	110.60
33	BA	1097	A	N1-C2-N3	-19.03	119.79	129.30
33	BA	2916	A	N1-C2-N3	-19.03	119.79	129.30
1	AA	671	A	C2-N3-C4	19.02	120.11	110.60
33	BA	305	A	C2-N3-C4	19.02	120.11	110.60
33	BA	2722	A	C2-N3-C4	19.02	120.11	110.60
33	BA	161	A	C2-N3-C4	19.02	120.11	110.60
33	BA	496	A	C2-N3-C4	19.02	120.11	110.60
33	BA	1392	A	C2-N3-C4	19.02	120.11	110.60
33	BA	867	A	C2-N3-C4	19.02	120.11	110.60
1	AA	506	A	C2-N3-C4	19.02	120.11	110.60
33	BA	64	A	N1-C2-N3	-19.02	119.79	129.30
33	BA	847	A	N1-C2-N3	-19.02	119.79	129.30
33	BA	1046	A	N1-C2-N3	-19.02	119.79	129.30
33	BA	407	A	C2-N3-C4	19.02	120.11	110.60
1	AA	649	A	C2-N3-C4	19.01	120.11	110.60
33	BA	925	A	N1-C2-N3	-19.01	119.79	129.30
33	BA	1778	A	C2-N3-C4	19.01	120.11	110.60
33	BA	342	A	C2-N3-C4	19.01	120.11	110.60
1	AA	899	A	N1-C2-N3	-19.01	119.80	129.30
33	BA	130	A	C2-N3-C4	19.01	120.11	110.60
33	BA	504	A	C2-N3-C4	19.01	120.11	110.60
33	BA	1700	A	C2-N3-C4	19.01	120.11	110.60
33	BA	2295	A	C2-N3-C4	19.01	120.11	110.60
33	BA	2754	A	C2-N3-C4	19.01	120.11	110.60
33	BA	44	A	C2-N3-C4	19.01	120.11	110.60
33	BA	965	A	C2-N3-C4	19.01	120.10	110.60
1	AA	55	A	C2-N3-C4	19.01	120.10	110.60
1	AA	658	A	C2-N3-C4	19.01	120.10	110.60
1	AA	775	A	C2-N3-C4	19.01	120.10	110.60
1	AA	1236	A	C2-N3-C4	19.00	120.10	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1355	A	N1-C2-N3	-19.00	119.80	129.30
33	BA	2117	A	C2-N3-C4	19.00	120.10	110.60
33	BA	1096	A	C2-N3-C4	19.00	120.10	110.60
33	BA	500	A	C2-N3-C4	19.00	120.10	110.60
1	AA	254	A	N1-C2-N3	-19.00	119.80	129.30
33	BA	1260	A	C2-N3-C4	19.00	120.10	110.60
1	AA	713	A	N1-C2-N3	-19.00	119.80	129.30
33	BA	758	A	C2-N3-C4	19.00	120.10	110.60
33	BA	1614	A	C2-N3-C4	19.00	120.10	110.60
33	BA	2262	A	N1-C2-N3	-19.00	119.80	129.30
1	AA	61	A	C2-N3-C4	18.99	120.10	110.60
1	AA	150	A	C2-N3-C4	18.99	120.10	110.60
33	BA	618	A	C2-N3-C4	18.99	120.10	110.60
33	BA	1814	A	N1-C2-N3	-18.99	119.80	129.30
1	AA	988	A	N1-C2-N3	-18.99	119.80	129.30
33	BA	530	A	C2-N3-C4	18.99	120.10	110.60
33	BA	952	A	C2-N3-C4	18.99	120.10	110.60
1	AA	208	A	C2-N3-C4	18.99	120.09	110.60
1	AA	381	A	C2-N3-C4	18.99	120.09	110.60
33	BA	2375	A	C2-N3-C4	18.99	120.09	110.60
1	AA	713	A	C2-N3-C4	18.99	120.09	110.60
33	BA	2898	A	C2-N3-C4	18.99	120.09	110.60
1	AA	1455	A	C2-N3-C4	18.98	120.09	110.60
33	BA	374	A	N1-C2-N3	-18.98	119.81	129.30
33	BA	652	A	C2-N3-C4	18.98	120.09	110.60
33	BA	2662	A	C2-N3-C4	18.98	120.09	110.60
1	AA	457	A	N1-C2-N3	-18.98	119.81	129.30
33	BA	2343	A	C2-N3-C4	18.98	120.09	110.60
33	BA	1417	A	C2-N3-C4	18.98	120.09	110.60
33	BA	1483	A	C2-N3-C4	18.98	120.09	110.60
33	BA	1914	A	C2-N3-C4	18.98	120.09	110.60
33	BA	1919	A	N1-C2-N3	-18.98	119.81	129.30
33	BA	1442	A	C2-N3-C4	18.98	120.09	110.60
33	BA	49	A	C2-N3-C4	18.97	120.09	110.60
1	AA	1342	A	C2-N3-C4	18.97	120.09	110.60
33	BA	2500	A	C2-N3-C4	18.97	120.09	110.60
1	AA	52	A	C2-N3-C4	18.97	120.08	110.60
1	AA	968	A	C2-N3-C4	18.97	120.08	110.60
33	BA	922	A	C2-N3-C4	18.97	120.08	110.60
33	BA	1126	A	C2-N3-C4	18.97	120.08	110.60
33	BA	1710	A	C2-N3-C4	18.97	120.08	110.60
1	AA	1213	A	C2-N3-C4	18.97	120.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	206	A	C2-N3-C4	18.97	120.08	110.60
33	BA	970	A	C2-N3-C4	18.97	120.08	110.60
1	AA	72	A	C2-N3-C4	18.97	120.08	110.60
33	BA	1243	A	C2-N3-C4	18.97	120.08	110.60
33	BA	1258	A	C2-N3-C4	18.97	120.08	110.60
1	AA	659	A	C2-N3-C4	18.96	120.08	110.60
1	AA	924	A	C2-N3-C4	18.96	120.08	110.60
33	BA	683	A	C2-N3-C4	18.96	120.08	110.60
33	BA	1473	A	C2-N3-C4	18.96	120.08	110.60
33	BA	2447	A	C2-N3-C4	18.96	120.08	110.60
33	BA	2790	A	C2-N3-C4	18.96	120.08	110.60
33	BA	318	A	C2-N3-C4	18.96	120.08	110.60
33	BA	2779	A	C2-N3-C4	18.96	120.08	110.60
1	AA	74	A	C2-N3-C4	18.96	120.08	110.60
33	BA	2089	A	N1-C2-N3	-18.96	119.82	129.30
1	AA	796	A	C2-N3-C4	18.96	120.08	110.60
33	BA	342	A	N1-C2-N3	-18.96	119.82	129.30
33	BA	418	A	C2-N3-C4	18.96	120.08	110.60
1	AA	1372	A	C2-N3-C4	18.96	120.08	110.60
21	AX	41	A	C2-N3-C4	18.96	120.08	110.60
33	BA	560	A	N1-C2-N3	-18.96	119.82	129.30
33	BA	2091	A	C2-N3-C4	18.96	120.08	110.60
34	BB	46	A	C2-N3-C4	18.96	120.08	110.60
1	AA	721	A	C2-N3-C4	18.95	120.08	110.60
1	AA	1349	A	C2-N3-C4	18.95	120.08	110.60
33	BA	61	A	C2-N3-C4	18.95	120.08	110.60
33	BA	1174	A	C2-N3-C4	18.95	120.08	110.60
33	BA	2026	A	C2-N3-C4	18.95	120.08	110.60
1	AA	397	A	C2-N3-C4	18.95	120.08	110.60
1	AA	415	A	N1-C2-N3	-18.95	119.82	129.30
33	BA	592	A	C2-N3-C4	18.95	120.08	110.60
33	BA	889	A	C2-N3-C4	18.95	120.08	110.60
33	BA	384	A	C2-N3-C4	18.95	120.08	110.60
34	BB	102	A	C2-N3-C4	18.95	120.08	110.60
1	AA	139	A	C2-N3-C4	18.95	120.08	110.60
33	BA	1601	A	C2-N3-C4	18.95	120.07	110.60
33	BA	2152	A	C2-N3-C4	18.95	120.08	110.60
33	BA	1123	A	C2-N3-C4	18.95	120.07	110.60
33	BA	1302	A	N1-C2-N3	-18.95	119.83	129.30
33	BA	1542	A	C2-N3-C4	18.95	120.07	110.60
1	AA	1320	A	C2-N3-C4	18.95	120.07	110.60
33	BA	429	A	C2-N3-C4	18.95	120.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1222	A	C2-N3-C4	18.95	120.07	110.60
33	BA	2042	A	C2-N3-C4	18.95	120.07	110.60
33	BA	2898	A	N1-C2-N3	-18.95	119.83	129.30
33	BA	593	A	N1-C2-N3	-18.95	119.83	129.30
1	AA	1298	A	C2-N3-C4	18.94	120.07	110.60
33	BA	2254	A	C2-N3-C4	18.94	120.07	110.60
1	AA	1407	A	N1-C2-N3	-18.94	119.83	129.30
33	BA	2670	A	N1-C2-N3	-18.94	119.83	129.30
21	AX	24	A	C2-N3-C4	18.94	120.07	110.60
33	BA	49	A	N1-C2-N3	-18.94	119.83	129.30
33	BA	2807	A	C2-N3-C4	18.94	120.07	110.60
1	AA	1486	A	C2-N3-C4	18.94	120.07	110.60
33	BA	1655	A	C2-N3-C4	18.94	120.07	110.60
33	BA	2769	A	C2-N3-C4	18.94	120.07	110.60
33	BA	2254	A	N1-C2-N3	-18.93	119.83	129.30
33	BA	1157	A	N1-C2-N3	-18.93	119.83	129.30
1	AA	382	A	C2-N3-C4	18.93	120.07	110.60
33	BA	364	A	C2-N3-C4	18.93	120.07	110.60
33	BA	2349	A	C2-N3-C4	18.93	120.07	110.60
33	BA	2845	A	C2-N3-C4	18.93	120.07	110.60
33	BA	56	A	C2-N3-C4	18.93	120.06	110.60
33	BA	870	A	C2-N3-C4	18.93	120.06	110.60
33	BA	1490	A	C2-N3-C4	18.93	120.06	110.60
33	BA	486	A	C2-N3-C4	18.93	120.06	110.60
33	BA	2560	A	C2-N3-C4	18.93	120.06	110.60
33	BA	2606	A	N1-C2-N3	-18.92	119.84	129.30
1	AA	512	A	C2-N3-C4	18.92	120.06	110.60
1	AA	985	A	N1-C2-N3	-18.92	119.84	129.30
1	AA	1517	A	C2-N3-C4	18.92	120.06	110.60
33	BA	171	A	C2-N3-C4	18.92	120.06	110.60
33	BA	2176	A	C2-N3-C4	18.92	120.06	110.60
33	BA	2402	A	C2-N3-C4	18.92	120.06	110.60
1	AA	390	A	C2-N3-C4	18.92	120.06	110.60
33	BA	326	A	C2-N3-C4	18.92	120.06	110.60
33	BA	634	A	C2-N3-C4	18.92	120.06	110.60
33	BA	1760	A	C2-N3-C4	18.92	120.06	110.60
33	BA	1999	A	C2-N3-C4	18.92	120.06	110.60
33	BA	2593	A	C2-N3-C4	18.92	120.06	110.60
33	BA	2834	A	C2-N3-C4	18.92	120.06	110.60
33	BA	2916	A	C2-N3-C4	18.92	120.06	110.60
1	AA	945	A	C2-N3-C4	18.92	120.06	110.60
33	BA	1210	A	C2-N3-C4	18.92	120.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	996	A	C2-N3-C4	18.92	120.06	110.60
1	AA	1355	A	C2-N3-C4	18.92	120.06	110.60
1	AA	1369	A	C2-N3-C4	18.92	120.06	110.60
33	BA	1269	A	C2-N3-C4	18.92	120.06	110.60
33	BA	2047	A	C2-N3-C4	18.92	120.06	110.60
33	BA	2902	A	C2-N3-C4	18.92	120.06	110.60
1	AA	669	A	C2-N3-C4	18.92	120.06	110.60
1	AA	703	A	N1-C2-N3	-18.92	119.84	129.30
1	AA	1185	A	C2-N3-C4	18.91	120.06	110.60
1	AA	1200	A	C2-N3-C4	18.91	120.06	110.60
1	AA	1435	A	C2-N3-C4	18.91	120.06	110.60
34	BB	18	A	C2-N3-C4	18.91	120.06	110.60
33	BA	882	A	C2-N3-C4	18.91	120.06	110.60
33	BA	1357	A	C2-N3-C4	18.91	120.06	110.60
1	AA	10	A	C2-N3-C4	18.91	120.06	110.60
1	AA	57	A	C2-N3-C4	18.91	120.06	110.60
1	AA	1259	A	C2-N3-C4	18.91	120.06	110.60
33	BA	28	A	C2-N3-C4	18.91	120.06	110.60
33	BA	216	A	C2-N3-C4	18.91	120.06	110.60
33	BA	1426	A	C2-N3-C4	18.91	120.06	110.60
33	BA	1636	A	C2-N3-C4	18.91	120.06	110.60
1	AA	1359	A	C2-N3-C4	18.91	120.05	110.60
33	BA	1617	A	C2-N3-C4	18.91	120.05	110.60
33	BA	1858	A	C2-N3-C4	18.91	120.05	110.60
1	AA	1425	A	C2-N3-C4	18.91	120.05	110.60
33	BA	2862	A	C2-N3-C4	18.91	120.05	110.60
1	AA	1327	A	C2-N3-C4	18.91	120.05	110.60
33	BA	658	A	C2-N3-C4	18.91	120.05	110.60
33	BA	2618	A	N1-C2-N3	-18.91	119.85	129.30
33	BA	2643	A	C2-N3-C4	18.91	120.05	110.60
33	BA	2762	A	C2-N3-C4	18.91	120.05	110.60
1	AA	440	A	C2-N3-C4	18.90	120.05	110.60
33	BA	1316	A	C2-N3-C4	18.90	120.05	110.60
1	AA	768	A	C2-N3-C4	18.90	120.05	110.60
1	AA	1189	A	C2-N3-C4	18.90	120.05	110.60
33	BA	6	A	C2-N3-C4	18.90	120.05	110.60
1	AA	1490	A	C2-N3-C4	18.90	120.05	110.60
33	BA	265	A	C2-N3-C4	18.90	120.05	110.60
33	BA	279	A	C2-N3-C4	18.90	120.05	110.60
33	BA	656	A	C2-N3-C4	18.90	120.05	110.60
33	BA	1340	A	C2-N3-C4	18.90	120.05	110.60
33	BA	1579	A	C2-N3-C4	18.90	120.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1914	A	N1-C2-N3	-18.90	119.85	129.30
33	BA	2700	A	C2-N3-C4	18.90	120.05	110.60
1	AA	899	A	C2-N3-C4	18.90	120.05	110.60
33	BA	1103	A	C2-N3-C4	18.90	120.05	110.60
33	BA	1685	A	C2-N3-C4	18.90	120.05	110.60
33	BA	637	A	C2-N3-C4	18.90	120.05	110.60
33	BA	1520	A	C2-N3-C4	18.90	120.05	110.60
33	BA	1814	A	C2-N3-C4	18.90	120.05	110.60
33	BA	2389	A	C2-N3-C4	18.90	120.05	110.60
33	BA	2480	A	C2-N3-C4	18.90	120.05	110.60
1	AA	870	A	C2-N3-C4	18.89	120.05	110.60
1	AA	1115	A	C2-N3-C4	18.89	120.05	110.60
1	AA	1523	A	C2-N3-C4	18.89	120.05	110.60
33	BA	494	A	N1-C2-N3	-18.89	119.85	129.30
33	BA	1042	A	N1-C2-N3	-18.89	119.85	129.30
33	BA	1188	A	N1-C2-N3	-18.89	119.85	129.30
33	BA	2165	A	C2-N3-C4	18.89	120.05	110.60
33	BA	1638	A	C2-N3-C4	18.89	120.05	110.60
33	BA	1713	A	N1-C2-N3	-18.89	119.85	129.30
33	BA	1813	A	C2-N3-C4	18.89	120.05	110.60
33	BA	1838	A	C2-N3-C4	18.89	120.05	110.60
33	BA	2134	A	C2-N3-C4	18.89	120.05	110.60
33	BA	2369	A	C2-N3-C4	18.89	120.05	110.60
33	BA	2375	A	N1-C2-N3	-18.89	119.85	129.30
1	AA	12	A	C2-N3-C4	18.89	120.05	110.60
1	AA	129	A	C2-N3-C4	18.89	120.05	110.60
1	AA	886	A	C2-N3-C4	18.89	120.05	110.60
33	BA	273	A	C2-N3-C4	18.89	120.05	110.60
1	AA	793	A	C2-N3-C4	18.89	120.04	110.60
1	AA	984	A	C2-N3-C4	18.89	120.05	110.60
1	AA	1509	A	C2-N3-C4	18.89	120.05	110.60
33	BA	724	A	C2-N3-C4	18.89	120.04	110.60
1	AA	775	A	N1-C2-N3	-18.89	119.86	129.30
33	BA	65	A	C2-N3-C4	18.89	120.04	110.60
33	BA	1189	A	N1-C2-N3	-18.89	119.86	129.30
33	BA	1918	A	C2-N3-C4	18.89	120.04	110.60
33	BA	2362	A	C2-N3-C4	18.89	120.04	110.60
1	AA	171	A	C2-N3-C4	18.89	120.04	110.60
1	AA	404	A	C2-N3-C4	18.89	120.04	110.60
33	BA	1202	A	C2-N3-C4	18.89	120.04	110.60
33	BA	2812	A	C2-N3-C4	18.89	120.04	110.60
33	BA	2889	A	C2-N3-C4	18.89	120.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	301	A	C2-N3-C4	18.88	120.04	110.60
1	AA	361	A	C2-N3-C4	18.88	120.04	110.60
33	BA	391	A	C2-N3-C4	18.88	120.04	110.60
33	BA	1709	A	C2-N3-C4	18.88	120.04	110.60
1	AA	148	A	C2-N3-C4	18.88	120.04	110.60
1	AA	389	A	C2-N3-C4	18.88	120.04	110.60
1	AA	529	A	C2-N3-C4	18.88	120.04	110.60
33	BA	683	A	N1-C2-N3	-18.88	119.86	129.30
33	BA	910	A	C2-N3-C4	18.88	120.04	110.60
33	BA	2100	A	C2-N3-C4	18.88	120.04	110.60
33	BA	2908	A	C2-N3-C4	18.88	120.04	110.60
33	BA	1325	A	C2-N3-C4	18.88	120.04	110.60
33	BA	2479	A	C2-N3-C4	18.88	120.04	110.60
1	AA	433	A	C2-N3-C4	18.88	120.04	110.60
1	AA	791	A	C2-N3-C4	18.88	120.04	110.60
33	BA	1340	A	N1-C2-N3	-18.88	119.86	129.30
1	AA	99	A	C2-N3-C4	18.88	120.04	110.60
1	AA	730	A	N1-C2-N3	-18.88	119.86	129.30
33	BA	1061	A	N1-C2-N3	-18.88	119.86	129.30
33	BA	2052	A	C2-N3-C4	18.88	120.04	110.60
1	AA	1166	A	C2-N3-C4	18.88	120.04	110.60
33	BA	345	A	C2-N3-C4	18.88	120.04	110.60
33	BA	1119	A	C2-N3-C4	18.88	120.04	110.60
33	BA	1424	A	C2-N3-C4	18.88	120.04	110.60
33	BA	1981	A	C2-N3-C4	18.88	120.04	110.60
33	BA	1995	A	C2-N3-C4	18.88	120.04	110.60
33	BA	2356	A	C2-N3-C4	18.88	120.04	110.60
33	BA	2907	A	C2-N3-C4	18.88	120.04	110.60
33	BA	71	A	C2-N3-C4	18.88	120.04	110.60
33	BA	118	A	N1-C2-N3	-18.88	119.86	129.30
33	BA	1945	A	C2-N3-C4	18.88	120.04	110.60
33	BA	2844	A	C2-N3-C4	18.88	120.04	110.60
1	AA	266	A	C2-N3-C4	18.87	120.04	110.60
1	AA	1179	A	C2-N3-C4	18.87	120.04	110.60
1	AA	1206	A	C2-N3-C4	18.87	120.04	110.60
1	AA	1470	A	C2-N3-C4	18.87	120.04	110.60
33	BA	224	A	C2-N3-C4	18.87	120.04	110.60
33	BA	479	A	C2-N3-C4	18.87	120.04	110.60
33	BA	2793	A	N1-C2-N3	-18.87	119.86	129.30
1	AA	271	A	C2-N3-C4	18.87	120.03	110.60
1	AA	1178	A	N1-C2-N3	-18.87	119.86	129.30
33	BA	118	A	C2-N3-C4	18.87	120.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	337	A	C2-N3-C4	18.87	120.03	110.60
33	BA	2302	A	C2-N3-C4	18.87	120.04	110.60
1	AA	211	A	C2-N3-C4	18.87	120.03	110.60
1	AA	190	A	C2-N3-C4	18.87	120.03	110.60
1	AA	251	A	C2-N3-C4	18.87	120.03	110.60
1	AA	582	A	C2-N3-C4	18.87	120.03	110.60
1	AA	1133	A	C2-N3-C4	18.87	120.03	110.60
33	BA	1142	A	C2-N3-C4	18.87	120.03	110.60
33	BA	2398	A	C2-N3-C4	18.87	120.03	110.60
33	BA	2663	A	C2-N3-C4	18.87	120.03	110.60
1	AA	240	A	C2-N3-C4	18.86	120.03	110.60
1	AA	1147	A	C2-N3-C4	18.86	120.03	110.60
21	AX	14	A	N1-C2-N3	-18.86	119.87	129.30
33	BA	896	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1556	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1919	A	C2-N3-C4	18.86	120.03	110.60
1	AA	522	A	C2-N3-C4	18.86	120.03	110.60
1	AA	824	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1583	A	C2-N3-C4	18.86	120.03	110.60
33	BA	2782	A	C2-N3-C4	18.86	120.03	110.60
1	AA	314	A	C2-N3-C4	18.86	120.03	110.60
1	AA	838	A	C2-N3-C4	18.86	120.03	110.60
1	AA	1488	A	C2-N3-C4	18.86	120.03	110.60
33	BA	21	A	C2-N3-C4	18.86	120.03	110.60
33	BA	388	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1132	A	N1-C2-N3	-18.86	119.87	129.30
33	BA	1235	A	C2-N3-C4	18.86	120.03	110.60
33	BA	2216	A	C2-N3-C4	18.86	120.03	110.60
33	BA	2252	A	C2-N3-C4	18.86	120.03	110.60
33	BA	222	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1008	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1161	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1312	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1555	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1672	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1677	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1784	A	C2-N3-C4	18.86	120.03	110.60
33	BA	2191	A	C2-N3-C4	18.86	120.03	110.60
33	BA	2507	A	C2-N3-C4	18.86	120.03	110.60
1	AA	617	A	C2-N3-C4	18.86	120.03	110.60
1	AA	677	A	C2-N3-C4	18.86	120.03	110.60
1	AA	925	A	C2-N3-C4	18.86	120.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1028	A	C2-N3-C4	18.86	120.03	110.60
33	BA	1233	A	C2-N3-C4	18.86	120.03	110.60
33	BA	2060	A	C2-N3-C4	18.86	120.03	110.60
33	BA	2708	A	N1-C2-N3	-18.86	119.87	129.30
1	AA	357	A	C2-N3-C4	18.86	120.03	110.60
33	BA	723	A	N1-C2-N3	-18.86	119.87	129.30
33	BA	2123	A	C2-N3-C4	18.86	120.03	110.60
33	BA	2893	A	C2-N3-C4	18.86	120.03	110.60
1	AA	225	A	C2-N3-C4	18.86	120.03	110.60
1	AA	1470	A	N1-C2-N3	-18.86	119.87	129.30
33	BA	225	A	C2-N3-C4	18.86	120.03	110.60
33	BA	999	A	C2-N3-C4	18.86	120.03	110.60
1	AA	281	A	C2-N3-C4	18.85	120.03	110.60
1	AA	978	A	C2-N3-C4	18.85	120.03	110.60
1	AA	1442	A	C2-N3-C4	18.85	120.03	110.60
33	BA	91	A	C2-N3-C4	18.85	120.03	110.60
33	BA	374	A	C2-N3-C4	18.85	120.03	110.60
33	BA	448	A	C2-N3-C4	18.85	120.03	110.60
33	BA	991	A	C2-N3-C4	18.85	120.03	110.60
33	BA	1265	A	C2-N3-C4	18.85	120.03	110.60
33	BA	2088	A	C2-N3-C4	18.85	120.03	110.60
33	BA	2170	A	C2-N3-C4	18.85	120.03	110.60
33	BA	2276	A	N1-C2-N3	-18.85	119.87	129.30
1	AA	685	A	C2-N3-C4	18.85	120.03	110.60
33	BA	173	A	C2-N3-C4	18.85	120.03	110.60
33	BA	1434	A	C2-N3-C4	18.85	120.03	110.60
33	BA	1876	A	C2-N3-C4	18.85	120.03	110.60
33	BA	1928	A	C2-N3-C4	18.85	120.03	110.60
33	BA	2629	A	C2-N3-C4	18.85	120.03	110.60
33	BA	2887	A	C2-N3-C4	18.85	120.03	110.60
1	AA	258	A	C2-N3-C4	18.85	120.03	110.60
1	AA	1502	A	C2-N3-C4	18.85	120.03	110.60
33	BA	762	A	C2-N3-C4	18.85	120.03	110.60
33	BA	1266	A	C2-N3-C4	18.85	120.03	110.60
33	BA	1797	A	C2-N3-C4	18.85	120.03	110.60
33	BA	2066	A	C2-N3-C4	18.85	120.03	110.60
33	BA	2511	A	C2-N3-C4	18.85	120.03	110.60
33	BA	957	A	N1-C2-N3	-18.85	119.88	129.30
33	BA	2317	A	C2-N3-C4	18.85	120.02	110.60
33	BA	2854	A	C2-N3-C4	18.85	120.02	110.60
1	AA	18	A	N1-C2-N3	-18.85	119.88	129.30
1	AA	452	A	C2-N3-C4	18.85	120.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	711	A	C2-N3-C4	18.85	120.02	110.60
1	AA	1272	A	C2-N3-C4	18.85	120.02	110.60
33	BA	207	A	N1-C2-N3	-18.85	119.88	129.30
33	BA	278	A	C2-N3-C4	18.85	120.02	110.60
33	BA	849	A	N1-C2-N3	-18.85	119.88	129.30
33	BA	1115	A	C2-N3-C4	18.85	120.02	110.60
33	BA	1601	A	N1-C2-N3	-18.85	119.88	129.30
33	BA	1713	A	C2-N3-C4	18.85	120.02	110.60
33	BA	2018	A	C2-N3-C4	18.85	120.02	110.60
33	BA	2141	A	C2-N3-C4	18.85	120.02	110.60
33	BA	2668	A	C2-N3-C4	18.85	120.02	110.60
33	BA	1284	A	C2-N3-C4	18.85	120.02	110.60
1	AA	94	A	C2-N3-C4	18.84	120.02	110.60
1	AA	371	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1111	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1261	A	N1-C2-N3	-18.84	119.88	129.30
33	BA	333	A	C2-N3-C4	18.84	120.02	110.60
33	BA	893	A	C2-N3-C4	18.84	120.02	110.60
33	BA	1026	A	C2-N3-C4	18.84	120.02	110.60
33	BA	1314	A	C2-N3-C4	18.84	120.02	110.60
33	BA	1375	A	C2-N3-C4	18.84	120.02	110.60
33	BA	1585	A	C2-N3-C4	18.84	120.02	110.60
33	BA	2205	A	C2-N3-C4	18.84	120.02	110.60
33	BA	2924	A	C2-N3-C4	18.84	120.02	110.60
1	AA	496	A	C2-N3-C4	18.84	120.02	110.60
1	AA	592	A	C2-N3-C4	18.84	120.02	110.60
1	AA	928	A	C2-N3-C4	18.84	120.02	110.60
33	BA	1593	A	C2-N3-C4	18.84	120.02	110.60
33	BA	2027	A	C2-N3-C4	18.84	120.02	110.60
33	BA	2658	A	C2-N3-C4	18.84	120.02	110.60
33	BA	2673	A	C2-N3-C4	18.84	120.02	110.60
33	BA	322	A	C2-N3-C4	18.84	120.02	110.60
33	BA	1313	A	C2-N3-C4	18.84	120.02	110.60
1	AA	10	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	140	A	C2-N3-C4	18.84	120.02	110.60
33	BA	5	A	C2-N3-C4	18.84	120.02	110.60
33	BA	125	A	C2-N3-C4	18.84	120.02	110.60
33	BA	476	A	C2-N3-C4	18.84	120.02	110.60
33	BA	1072	A	C2-N3-C4	18.84	120.02	110.60
33	BA	1691	A	N1-C2-N3	-18.84	119.88	129.30
33	BA	1844	A	N1-C2-N3	-18.84	119.88	129.30
33	BA	2298	A	C2-N3-C4	18.84	120.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	715	A	C2-N3-C4	18.84	120.02	110.60
1	AA	979	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1419	A	C2-N3-C4	18.84	120.02	110.60
33	BA	154	A	C2-N3-C4	18.84	120.02	110.60
33	BA	210	A	C2-N3-C4	18.84	120.02	110.60
33	BA	647	A	N1-C2-N3	-18.84	119.88	129.30
33	BA	1532	A	C2-N3-C4	18.84	120.02	110.60
1	AA	837	A	C2-N3-C4	18.84	120.02	110.60
1	AA	1120	A	C2-N3-C4	18.84	120.02	110.60
33	BA	421	A	C2-N3-C4	18.84	120.02	110.60
33	BA	702	A	C2-N3-C4	18.84	120.02	110.60
33	BA	830	A	C2-N3-C4	18.84	120.02	110.60
33	BA	1194	A	C2-N3-C4	18.84	120.02	110.60
33	BA	2132	A	C2-N3-C4	18.84	120.02	110.60
33	BA	2270	A	C2-N3-C4	18.84	120.02	110.60
33	BA	2686	A	C2-N3-C4	18.84	120.02	110.60
33	BA	2893	A	N1-C2-N3	-18.84	119.88	129.30
34	BB	39	A	C2-N3-C4	18.84	120.02	110.60
1	AA	206	A	C2-N3-C4	18.83	120.02	110.60
33	BA	325	A	C2-N3-C4	18.83	120.02	110.60
33	BA	894	A	C2-N3-C4	18.83	120.02	110.60
33	BA	1592	A	C2-N3-C4	18.83	120.02	110.60
33	BA	1653	A	C2-N3-C4	18.83	120.02	110.60
1	AA	462	A	C2-N3-C4	18.83	120.02	110.60
1	AA	491	A	C2-N3-C4	18.83	120.02	110.60
33	BA	110	A	C2-N3-C4	18.83	120.02	110.60
33	BA	193	A	C2-N3-C4	18.83	120.02	110.60
33	BA	1287	A	C2-N3-C4	18.83	120.02	110.60
33	BA	1325	A	N1-C2-N3	-18.83	119.88	129.30
33	BA	1553	A	C2-N3-C4	18.83	120.02	110.60
33	BA	1675	A	C2-N3-C4	18.83	120.02	110.60
33	BA	1776	A	C2-N3-C4	18.83	120.02	110.60
1	AA	1308	A	N1-C2-N3	-18.83	119.88	129.30
33	BA	95	A	C2-N3-C4	18.83	120.02	110.60
33	BA	690	A	C2-N3-C4	18.83	120.02	110.60
33	BA	821	A	C2-N3-C4	18.83	120.02	110.60
33	BA	888	A	C2-N3-C4	18.83	120.02	110.60
34	BB	114	A	C2-N3-C4	18.83	120.02	110.60
1	AA	548	A	C2-N3-C4	18.83	120.02	110.60
1	AA	605	A	C2-N3-C4	18.83	120.02	110.60
1	AA	1092	A	C2-N3-C4	18.83	120.02	110.60
33	BA	1588	A	C2-N3-C4	18.83	120.01	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1663	A	C2-N3-C4	18.83	120.02	110.60
33	BA	1774	A	C2-N3-C4	18.83	120.02	110.60
33	BA	1848	A	C2-N3-C4	18.83	120.02	110.60
33	BA	2570	A	C2-N3-C4	18.83	120.02	110.60
33	BA	2594	A	C2-N3-C4	18.83	120.02	110.60
33	BA	2900	A	C2-N3-C4	18.83	120.02	110.60
34	BB	11	A	N1-C2-N3	-18.83	119.89	129.30
1	AA	364	A	C2-N3-C4	18.83	120.01	110.60
1	AA	801	A	C2-N3-C4	18.83	120.01	110.60
33	BA	73	A	C2-N3-C4	18.83	120.01	110.60
1	AA	664	A	C2-N3-C4	18.83	120.01	110.60
33	BA	431	A	C2-N3-C4	18.83	120.01	110.60
33	BA	507	A	C2-N3-C4	18.83	120.01	110.60
33	BA	2851	A	C2-N3-C4	18.83	120.01	110.60
1	AA	278	A	C2-N3-C4	18.82	120.01	110.60
1	AA	456	A	C2-N3-C4	18.82	120.01	110.60
1	AA	1140	A	C2-N3-C4	18.82	120.01	110.60
1	AA	1188	A	C2-N3-C4	18.82	120.01	110.60
21	AX	21	A	C2-N3-C4	18.82	120.01	110.60
33	BA	176	A	C2-N3-C4	18.82	120.01	110.60
33	BA	219	A	C2-N3-C4	18.82	120.01	110.60
33	BA	770	A	C2-N3-C4	18.82	120.01	110.60
33	BA	1347	A	N1-C2-N3	-18.82	119.89	129.30
33	BA	1746	A	C2-N3-C4	18.82	120.01	110.60
33	BA	2704	A	C2-N3-C4	18.82	120.01	110.60
33	BA	2908	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	440	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	776	A	C2-N3-C4	18.82	120.01	110.60
33	BA	2007	A	C2-N3-C4	18.82	120.01	110.60
1	AA	544	A	C2-N3-C4	18.82	120.01	110.60
21	AX	44	A	C2-N3-C4	18.82	120.01	110.60
33	BA	548	A	C2-N3-C4	18.82	120.01	110.60
33	BA	790	A	C2-N3-C4	18.82	120.01	110.60
33	BA	1784	A	N1-C2-N3	-18.82	119.89	129.30
33	BA	1789	A	C2-N3-C4	18.82	120.01	110.60
33	BA	2030	A	C2-N3-C4	18.82	120.01	110.60
33	BA	2124	A	C2-N3-C4	18.82	120.01	110.60
33	BA	2358	A	C2-N3-C4	18.82	120.01	110.60
33	BA	1189	A	C2-N3-C4	18.82	120.01	110.60
33	BA	1244	A	C2-N3-C4	18.82	120.01	110.60
33	BA	1347	A	C2-N3-C4	18.82	120.01	110.60
33	BA	2088	A	N1-C2-N3	-18.82	119.89	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	148	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	724	A	C2-N3-C4	18.82	120.01	110.60
1	AA	762	A	C2-N3-C4	18.82	120.01	110.60
33	BA	28	A	N1-C2-N3	-18.82	119.89	129.30
33	BA	389	A	C2-N3-C4	18.82	120.01	110.60
33	BA	999	A	N1-C2-N3	-18.82	119.89	129.30
33	BA	1036	A	C2-N3-C4	18.82	120.01	110.60
33	BA	1461	A	C2-N3-C4	18.82	120.01	110.60
33	BA	1631	A	C2-N3-C4	18.82	120.01	110.60
33	BA	2146	A	C2-N3-C4	18.82	120.01	110.60
33	BA	2295	A	N1-C2-N3	-18.82	119.89	129.30
33	BA	2338	A	C2-N3-C4	18.82	120.01	110.60
1	AA	202	A	C2-N3-C4	18.82	120.01	110.60
1	AA	333	A	C2-N3-C4	18.82	120.01	110.60
1	AA	1121	A	C2-N3-C4	18.82	120.01	110.60
33	BA	659	A	N1-C2-N3	-18.82	119.89	129.30
33	BA	1844	A	C2-N3-C4	18.82	120.01	110.60
33	BA	2000	A	C2-N3-C4	18.82	120.01	110.60
1	AA	159	A	C2-N3-C4	18.82	120.01	110.60
1	AA	500	A	C2-N3-C4	18.82	120.01	110.60
1	AA	690	A	C2-N3-C4	18.82	120.01	110.60
1	AA	1205	A	C2-N3-C4	18.82	120.01	110.60
1	AA	1403	A	C2-N3-C4	18.82	120.01	110.60
1	AA	1463	A	C2-N3-C4	18.82	120.01	110.60
33	BA	207	A	C2-N3-C4	18.82	120.01	110.60
33	BA	275	A	C2-N3-C4	18.82	120.01	110.60
33	BA	456	A	C2-N3-C4	18.82	120.01	110.60
33	BA	578	A	C2-N3-C4	18.82	120.01	110.60
33	BA	653	A	C2-N3-C4	18.82	120.01	110.60
33	BA	1055	A	C2-N3-C4	18.82	120.01	110.60
33	BA	1277	A	C2-N3-C4	18.82	120.01	110.60
33	BA	1579	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	743	A	C2-N3-C4	18.81	120.01	110.60
1	AA	828	A	C2-N3-C4	18.81	120.01	110.60
33	BA	139	A	N1-C2-N3	-18.81	119.89	129.30
33	BA	139	A	C2-N3-C4	18.81	120.01	110.60
33	BA	705	A	C2-N3-C4	18.81	120.01	110.60
33	BA	1305	A	C2-N3-C4	18.81	120.01	110.60
33	BA	1381	A	C2-N3-C4	18.81	120.01	110.60
1	AA	459	A	C2-N3-C4	18.81	120.01	110.60
1	AA	910	A	C2-N3-C4	18.81	120.01	110.60
1	AA	1405	A	C2-N3-C4	18.81	120.01	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	144	A	C2-N3-C4	18.81	120.01	110.60
33	BA	449	A	C2-N3-C4	18.81	120.01	110.60
33	BA	1027	A	C2-N3-C4	18.81	120.01	110.60
33	BA	1144	A	C2-N3-C4	18.81	120.01	110.60
33	BA	2034	A	C2-N3-C4	18.81	120.01	110.60
33	BA	2461	A	C2-N3-C4	18.81	120.01	110.60
33	BA	2507	A	N1-C2-N3	-18.81	119.89	129.30
33	BA	2778	A	C2-N3-C4	18.81	120.01	110.60
33	BA	2830	A	C2-N3-C4	18.81	120.01	110.60
34	BB	25	A	C2-N3-C4	18.81	120.01	110.60
1	AA	234	A	C2-N3-C4	18.81	120.00	110.60
33	BA	412	A	C2-N3-C4	18.81	120.01	110.60
33	BA	549	A	C2-N3-C4	18.81	120.00	110.60
33	BA	769	A	C2-N3-C4	18.81	120.01	110.60
33	BA	851	A	C2-N3-C4	18.81	120.00	110.60
1	AA	28	A	C2-N3-C4	18.81	120.00	110.60
1	AA	1541	A	C2-N3-C4	18.81	120.00	110.60
33	BA	102	A	C2-N3-C4	18.81	120.00	110.60
33	BA	161	A	N1-C2-N3	-18.81	119.89	129.30
33	BA	947	A	C2-N3-C4	18.81	120.00	110.60
33	BA	1695	A	C2-N3-C4	18.81	120.00	110.60
1	AA	254	A	C2-N3-C4	18.81	120.00	110.60
1	AA	919	A	C2-N3-C4	18.81	120.00	110.60
33	BA	247	A	C2-N3-C4	18.81	120.00	110.60
33	BA	1254	A	C2-N3-C4	18.81	120.00	110.60
33	BA	1423	A	C2-N3-C4	18.81	120.00	110.60
34	BB	44	A	C2-N3-C4	18.81	120.00	110.60
34	BB	71	A	N1-C2-N3	-18.81	119.90	129.30
1	AA	228	A	C2-N3-C4	18.81	120.00	110.60
1	AA	438	A	C2-N3-C4	18.81	120.00	110.60
1	AA	913	A	C2-N3-C4	18.81	120.00	110.60
1	AA	1016	A	C2-N3-C4	18.81	120.00	110.60
33	BA	692	A	C2-N3-C4	18.81	120.00	110.60
33	BA	2087	A	C2-N3-C4	18.81	120.00	110.60
33	BA	2767	A	C2-N3-C4	18.81	120.00	110.60
34	BB	25	A	N1-C2-N3	-18.81	119.90	129.30
1	AA	142	A	C2-N3-C4	18.80	120.00	110.60
1	AA	506	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	651	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1271	A	C2-N3-C4	18.80	120.00	110.60
33	BA	547	A	C2-N3-C4	18.80	120.00	110.60
33	BA	978	A	C2-N3-C4	18.80	120.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1465	A	C2-N3-C4	18.80	120.00	110.60
1	AA	31	A	C2-N3-C4	18.80	120.00	110.60
1	AA	475	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1510	A	C2-N3-C4	18.80	120.00	110.60
33	BA	200	A	C2-N3-C4	18.80	120.00	110.60
33	BA	268	A	C2-N3-C4	18.80	120.00	110.60
33	BA	274	A	C2-N3-C4	18.80	120.00	110.60
33	BA	324	A	C2-N3-C4	18.80	120.00	110.60
33	BA	1230	A	C2-N3-C4	18.80	120.00	110.60
33	BA	1654	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2479	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	1022	A	C2-N3-C4	18.80	120.00	110.60
33	BA	231	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2316	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1266	A	C2-N3-C4	18.80	120.00	110.60
33	BA	677	A	C2-N3-C4	18.80	120.00	110.60
33	BA	1179	A	C2-N3-C4	18.80	120.00	110.60
33	BA	1906	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2227	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2477	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2505	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2719	A	C2-N3-C4	18.80	120.00	110.60
1	AA	35	A	C2-N3-C4	18.80	120.00	110.60
1	AA	173	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1128	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1234	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	1256	A	C2-N3-C4	18.80	120.00	110.60
33	BA	314	A	N1-C2-N3	-18.80	119.90	129.30
33	BA	1036	A	N1-C2-N3	-18.80	119.90	129.30
33	BA	1504	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2327	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2860	A	C2-N3-C4	18.80	120.00	110.60
1	AA	208	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	423	A	C2-N3-C4	18.80	120.00	110.60
33	BA	373	A	C2-N3-C4	18.80	120.00	110.60
33	BA	475	A	N1-C2-N3	-18.80	119.90	129.30
33	BA	1059	A	C2-N3-C4	18.80	120.00	110.60
33	BA	1432	A	N1-C2-N3	-18.80	119.90	129.30
33	BA	1456	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2262	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2767	A	N1-C2-N3	-18.80	119.90	129.30
33	BA	2787	A	C2-N3-C4	18.80	120.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2831	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2869	A	C2-N3-C4	18.80	120.00	110.60
1	AA	1528	A	C2-N3-C4	18.80	120.00	110.60
33	BA	229	A	C2-N3-C4	18.80	120.00	110.60
33	BA	659	A	C2-N3-C4	18.80	120.00	110.60
33	BA	821	A	N1-C2-N3	-18.80	119.90	129.30
33	BA	1723	A	C2-N3-C4	18.80	120.00	110.60
33	BA	1965	A	C2-N3-C4	18.80	120.00	110.60
33	BA	2398	A	N1-C2-N3	-18.80	119.90	129.30
33	BA	2819	A	N1-C2-N3	-18.80	119.90	129.30
34	BB	64	A	C2-N3-C4	18.80	120.00	110.60
1	AA	879	A	N1-C2-N3	-18.79	119.90	129.30
33	BA	1845	A	C2-N3-C4	18.79	120.00	110.60
33	BA	2119	A	C2-N3-C4	18.79	120.00	110.60
1	AA	321	A	N1-C2-N3	-18.79	119.90	129.30
1	AA	381	A	N1-C2-N3	-18.79	119.90	129.30
1	AA	1056	A	C2-N3-C4	18.79	120.00	110.60
1	AA	1260	A	N1-C2-N3	-18.79	119.90	129.30
1	AA	1386	A	C2-N3-C4	18.79	120.00	110.60
21	AX	70	A	C2-N3-C4	18.79	120.00	110.60
33	BA	64	A	C2-N3-C4	18.79	120.00	110.60
33	BA	302	A	C2-N3-C4	18.79	120.00	110.60
33	BA	307	A	C2-N3-C4	18.79	120.00	110.60
33	BA	618	A	N1-C2-N3	-18.79	119.90	129.30
33	BA	619	A	C2-N3-C4	18.79	120.00	110.60
33	BA	2734	A	C2-N3-C4	18.79	120.00	110.60
1	AA	372	A	C2-N3-C4	18.79	120.00	110.60
1	AA	1112	A	C2-N3-C4	18.79	120.00	110.60
1	AA	1205	A	N1-C2-N3	-18.79	119.90	129.30
33	BA	418	A	N1-C2-N3	-18.79	119.91	129.30
33	BA	616	A	C2-N3-C4	18.79	120.00	110.60
33	BA	2357	A	C2-N3-C4	18.79	120.00	110.60
34	BB	27	A	C2-N3-C4	18.79	120.00	110.60
34	BB	113	A	C2-N3-C4	18.79	120.00	110.60
1	AA	422	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	485	A	C2-N3-C4	18.79	120.00	110.60
1	AA	581	A	C2-N3-C4	18.79	119.99	110.60
1	AA	592	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	803	A	C2-N3-C4	18.79	120.00	110.60
1	AA	816	A	C2-N3-C4	18.79	120.00	110.60
33	BA	524	A	C2-N3-C4	18.79	120.00	110.60
33	BA	1025	A	C2-N3-C4	18.79	120.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1326	A	C2-N3-C4	18.79	120.00	110.60
33	BA	1445	A	C2-N3-C4	18.79	119.99	110.60
33	BA	1480	A	N1-C2-N3	-18.79	119.91	129.30
33	BA	1967	A	C2-N3-C4	18.79	120.00	110.60
33	BA	2276	A	C2-N3-C4	18.79	120.00	110.60
33	BA	2517	A	C2-N3-C4	18.79	120.00	110.60
33	BA	2750	A	C2-N3-C4	18.79	119.99	110.60
1	AA	611	A	C2-N3-C4	18.79	119.99	110.60
33	BA	140	A	C2-N3-C4	18.79	119.99	110.60
33	BA	1029	A	N1-C2-N3	-18.79	119.91	129.30
33	BA	1802	A	C2-N3-C4	18.79	119.99	110.60
33	BA	1956	A	C2-N3-C4	18.79	119.99	110.60
33	BA	2571	A	C2-N3-C4	18.79	119.99	110.60
1	AA	419	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	776	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	1222	A	C2-N3-C4	18.79	119.99	110.60
1	AA	1270	A	C2-N3-C4	18.79	119.99	110.60
1	AA	1289	A	N1-C2-N3	-18.79	119.91	129.30
33	BA	575	A	N1-C2-N3	-18.79	119.91	129.30
33	BA	774	A	C2-N3-C4	18.79	119.99	110.60
33	BA	956	A	C2-N3-C4	18.79	119.99	110.60
33	BA	1116	A	C2-N3-C4	18.79	119.99	110.60
33	BA	1308	A	C2-N3-C4	18.79	119.99	110.60
33	BA	1499	A	C2-N3-C4	18.79	119.99	110.60
33	BA	1816	A	C2-N3-C4	18.79	119.99	110.60
33	BA	2468	A	C2-N3-C4	18.79	119.99	110.60
1	AA	422	A	C2-N3-C4	18.79	119.99	110.60
1	AA	438	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	1488	A	N1-C2-N3	-18.79	119.91	129.30
33	BA	94	A	C2-N3-C4	18.79	119.99	110.60
33	BA	156	A	C2-N3-C4	18.79	119.99	110.60
33	BA	2462	A	C2-N3-C4	18.79	119.99	110.60
33	BA	2848	A	N1-C2-N3	-18.79	119.91	129.30
34	BB	51	A	C2-N3-C4	18.79	119.99	110.60
1	AA	500	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	875	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1133	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	1210	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1247	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1451	A	C2-N3-C4	18.78	119.99	110.60
33	BA	12	A	C2-N3-C4	18.78	119.99	110.60
33	BA	230	A	C2-N3-C4	18.78	119.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	329	A	C2-N3-C4	18.78	119.99	110.60
33	BA	369	A	C2-N3-C4	18.78	119.99	110.60
33	BA	600	A	C2-N3-C4	18.78	119.99	110.60
33	BA	619	A	N1-C2-N3	-18.78	119.91	129.30
33	BA	753	A	C2-N3-C4	18.78	119.99	110.60
33	BA	847	A	C2-N3-C4	18.78	119.99	110.60
33	BA	1406	A	C2-N3-C4	18.78	119.99	110.60
33	BA	2417	A	C2-N3-C4	18.78	119.99	110.60
33	BA	2464	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1180	A	C2-N3-C4	18.78	119.99	110.60
33	BA	314	A	C2-N3-C4	18.78	119.99	110.60
33	BA	1506	A	N1-C2-N3	-18.78	119.91	129.30
33	BA	1575	A	C2-N3-C4	18.78	119.99	110.60
33	BA	2590	A	C2-N3-C4	18.78	119.99	110.60
33	BA	2876	A	C2-N3-C4	18.78	119.99	110.60
34	BB	44	A	N1-C2-N3	-18.78	119.91	129.30
34	BB	102	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	171	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	825	A	C2-N3-C4	18.78	119.99	110.60
1	AA	874	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1437	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1479	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1529	A	C2-N3-C4	18.78	119.99	110.60
33	BA	584	A	C2-N3-C4	18.78	119.99	110.60
33	BA	699	A	C2-N3-C4	18.78	119.99	110.60
33	BA	774	A	N1-C2-N3	-18.78	119.91	129.30
33	BA	1533	A	C2-N3-C4	18.78	119.99	110.60
33	BA	2436	A	C2-N3-C4	18.78	119.99	110.60
34	BB	99	A	C2-N3-C4	18.78	119.99	110.60
1	AA	556	A	C2-N3-C4	18.78	119.99	110.60
1	AA	737	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	947	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1512	A	N1-C2-N3	-18.78	119.91	129.30
33	BA	71	A	N1-C2-N3	-18.78	119.91	129.30
33	BA	436	A	C2-N3-C4	18.78	119.99	110.60
33	BA	1141	A	C2-N3-C4	18.78	119.99	110.60
33	BA	1516	A	C2-N3-C4	18.78	119.99	110.60
1	AA	346	A	C2-N3-C4	18.78	119.99	110.60
1	AA	902	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1017	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1065	A	C2-N3-C4	18.78	119.99	110.60
1	AA	1200	A	N1-C2-N3	-18.78	119.91	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1261	A	C2-N3-C4	18.78	119.99	110.60
33	BA	575	A	C2-N3-C4	18.78	119.99	110.60
33	BA	1269	A	N1-C2-N3	-18.78	119.91	129.30
33	BA	1346	A	C2-N3-C4	18.78	119.99	110.60
33	BA	1361	A	C2-N3-C4	18.78	119.99	110.60
33	BA	2819	A	C2-N3-C4	18.78	119.99	110.60
1	AA	730	A	C2-N3-C4	18.78	119.99	110.60
33	BA	2708	A	C2-N3-C4	18.78	119.99	110.60
34	BB	50	A	C2-N3-C4	18.78	119.99	110.60
1	AA	67	A	C2-N3-C4	18.77	119.99	110.60
1	AA	811	A	C2-N3-C4	18.77	119.99	110.60
1	AA	968	A	N1-C2-N3	-18.77	119.91	129.30
33	BA	124	A	C2-N3-C4	18.77	119.99	110.60
33	BA	1335	A	C2-N3-C4	18.77	119.99	110.60
33	BA	2740	A	C2-N3-C4	18.77	119.99	110.60
1	AA	1257	A	C2-N3-C4	18.77	119.99	110.60
33	BA	10	A	C2-N3-C4	18.77	119.99	110.60
33	BA	470	A	C2-N3-C4	18.77	119.99	110.60
33	BA	572	A	C2-N3-C4	18.77	119.99	110.60
33	BA	808	A	C2-N3-C4	18.77	119.99	110.60
33	BA	1131	A	C2-N3-C4	18.77	119.99	110.60
33	BA	1699	A	C2-N3-C4	18.77	119.99	110.60
33	BA	2618	A	C2-N3-C4	18.77	119.99	110.60
1	AA	195	A	N1-C2-N3	-18.77	119.91	129.30
1	AA	204	A	C2-N3-C4	18.77	119.99	110.60
1	AA	270	A	C2-N3-C4	18.77	119.99	110.60
1	AA	296	A	C2-N3-C4	18.77	119.99	110.60
1	AA	777	A	C2-N3-C4	18.77	119.99	110.60
1	AA	791	A	N1-C2-N3	-18.77	119.91	129.30
1	AA	948	A	C2-N3-C4	18.77	119.99	110.60
1	AA	1383	A	C2-N3-C4	18.77	119.99	110.60
21	AX	58	A	C2-N3-C4	18.77	119.99	110.60
33	BA	244	A	C2-N3-C4	18.77	119.98	110.60
33	BA	476	A	N1-C2-N3	-18.77	119.91	129.30
33	BA	1266	A	N1-C2-N3	-18.77	119.91	129.30
33	BA	1913	A	C2-N3-C4	18.77	119.99	110.60
33	BA	2810	A	N1-C2-N3	-18.77	119.91	129.30
34	BB	20	A	C2-N3-C4	18.77	119.98	110.60
33	BA	477	A	N1-C2-N3	-18.77	119.92	129.30
33	BA	1679	A	C2-N3-C4	18.77	119.98	110.60
33	BA	1930	A	N1-C2-N3	-18.77	119.92	129.30
33	BA	2793	A	C2-N3-C4	18.77	119.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	39	A	N1-C2-N3	-18.77	119.92	129.30
1	AA	1289	A	C2-N3-C4	18.77	119.98	110.60
33	BA	226	A	N1-C2-N3	-18.77	119.92	129.30
33	BA	462	A	C2-N3-C4	18.77	119.98	110.60
33	BA	723	A	C2-N3-C4	18.77	119.98	110.60
33	BA	763	A	C2-N3-C4	18.77	119.98	110.60
33	BA	1092	A	C2-N3-C4	18.77	119.98	110.60
33	BA	1113	A	C2-N3-C4	18.77	119.98	110.60
33	BA	2683	A	C2-N3-C4	18.77	119.98	110.60
1	AA	474	A	C2-N3-C4	18.77	119.98	110.60
1	AA	616	A	C2-N3-C4	18.77	119.98	110.60
1	AA	917	A	C2-N3-C4	18.77	119.98	110.60
1	AA	1252	A	C2-N3-C4	18.77	119.98	110.60
33	BA	1735	A	C2-N3-C4	18.77	119.98	110.60
33	BA	2059	A	N1-C2-N3	-18.77	119.92	129.30
33	BA	2220	A	C2-N3-C4	18.77	119.98	110.60
33	BA	2837	A	C2-N3-C4	18.77	119.98	110.60
1	AA	236	A	C2-N3-C4	18.77	119.98	110.60
33	BA	702	A	N1-C2-N3	-18.77	119.92	129.30
33	BA	987	A	C2-N3-C4	18.77	119.98	110.60
33	BA	1743	A	C2-N3-C4	18.77	119.98	110.60
33	BA	2482	A	C2-N3-C4	18.77	119.98	110.60
33	BA	2923	A	C2-N3-C4	18.77	119.98	110.60
1	AA	1054	A	C2-N3-C4	18.76	119.98	110.60
33	BA	259	A	C2-N3-C4	18.76	119.98	110.60
33	BA	1224	A	C2-N3-C4	18.76	119.98	110.60
33	BA	1534	A	C2-N3-C4	18.76	119.98	110.60
33	BA	2071	A	C2-N3-C4	18.76	119.98	110.60
33	BA	2362	A	N1-C2-N3	-18.76	119.92	129.30
33	BA	2875	A	C2-N3-C4	18.76	119.98	110.60
1	AA	638	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1014	A	C2-N3-C4	18.76	119.98	110.60
33	BA	126	A	N1-C2-N3	-18.76	119.92	129.30
33	BA	1100	A	C2-N3-C4	18.76	119.98	110.60
33	BA	1813	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	178	A	C2-N3-C4	18.76	119.98	110.60
1	AA	321	A	C2-N3-C4	18.76	119.98	110.60
1	AA	542	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	924	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	1254	A	C2-N3-C4	18.76	119.98	110.60
1	AA	1434	A	C2-N3-C4	18.76	119.98	110.60
33	BA	1061	A	C2-N3-C4	18.76	119.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1686	A	C2-N3-C4	18.76	119.98	110.60
33	BA	2148	A	C2-N3-C4	18.76	119.98	110.60
33	BA	2365	A	C2-N3-C4	18.76	119.98	110.60
33	BA	2547	A	N1-C2-N3	-18.76	119.92	129.30
33	BA	622	A	C2-N3-C4	18.76	119.98	110.60
33	BA	2661	A	C2-N3-C4	18.76	119.98	110.60
1	AA	386	A	C2-N3-C4	18.76	119.98	110.60
1	AA	837	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	1090	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	1455	A	N1-C2-N3	-18.76	119.92	129.30
33	BA	459	A	C2-N3-C4	18.76	119.98	110.60
33	BA	876	A	C2-N3-C4	18.76	119.98	110.60
33	BA	908	A	C2-N3-C4	18.76	119.98	110.60
33	BA	1005	A	N1-C2-N3	-18.76	119.92	129.30
33	BA	1925	A	C2-N3-C4	18.76	119.98	110.60
33	BA	2482	A	N1-C2-N3	-18.76	119.92	129.30
33	BA	2498	A	C2-N3-C4	18.76	119.98	110.60
33	BA	2532	A	N1-C2-N3	-18.76	119.92	129.30
33	BA	2904	A	C2-N3-C4	18.76	119.98	110.60
1	AA	401	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	925	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	933	A	C2-N3-C4	18.76	119.98	110.60
33	BA	1680	A	C2-N3-C4	18.76	119.98	110.60
33	BA	2480	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	76	A	C2-N3-C4	18.75	119.98	110.60
1	AA	501	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	544	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	786	A	C2-N3-C4	18.75	119.98	110.60
1	AA	1024	A	C2-N3-C4	18.75	119.98	110.60
33	BA	494	A	C2-N3-C4	18.75	119.98	110.60
33	BA	1491	A	N1-C2-N3	-18.75	119.92	129.30
33	BA	1627	A	C2-N3-C4	18.75	119.98	110.60
33	BA	1961	A	C2-N3-C4	18.75	119.98	110.60
33	BA	2018	A	N1-C2-N3	-18.75	119.92	129.30
33	BA	2256	A	C2-N3-C4	18.75	119.98	110.60
33	BA	2307	A	C2-N3-C4	18.75	119.98	110.60
33	BA	2497	A	C2-N3-C4	18.75	119.98	110.60
1	AA	306	A	C2-N3-C4	18.75	119.98	110.60
1	AA	337	A	C2-N3-C4	18.75	119.98	110.60
1	AA	1427	A	C2-N3-C4	18.75	119.98	110.60
33	BA	1141	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	170	A	N1-C2-N3	-18.75	119.92	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1298	A	N1-C2-N3	-18.75	119.92	129.30
33	BA	428	A	C2-N3-C4	18.75	119.97	110.60
33	BA	551	A	C2-N3-C4	18.75	119.98	110.60
33	BA	781	A	C2-N3-C4	18.75	119.98	110.60
33	BA	782	A	C2-N3-C4	18.75	119.97	110.60
33	BA	1014	A	C2-N3-C4	18.75	119.97	110.60
33	BA	1323	A	C2-N3-C4	18.75	119.98	110.60
33	BA	1697	A	C2-N3-C4	18.75	119.98	110.60
33	BA	2406	A	C2-N3-C4	18.75	119.98	110.60
33	BA	2683	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	206	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	1284	A	C2-N3-C4	18.75	119.97	110.60
33	BA	991	A	N1-C2-N3	-18.75	119.92	129.30
33	BA	1615	A	C2-N3-C4	18.75	119.97	110.60
33	BA	2777	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	344	A	C2-N3-C4	18.75	119.97	110.60
1	AA	367	A	C2-N3-C4	18.75	119.97	110.60
1	AA	771	A	C2-N3-C4	18.75	119.97	110.60
1	AA	1050	A	C2-N3-C4	18.75	119.97	110.60
1	AA	1207	A	N1-C2-N3	-18.75	119.92	129.30
33	BA	1405	A	C2-N3-C4	18.75	119.97	110.60
33	BA	1608	A	C2-N3-C4	18.75	119.97	110.60
33	BA	2200	A	C2-N3-C4	18.75	119.97	110.60
33	BA	2876	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	306	A	N1-C2-N3	-18.75	119.93	129.30
33	BA	198	A	C2-N3-C4	18.75	119.97	110.60
33	BA	305	A	N1-C2-N3	-18.75	119.93	129.30
33	BA	376	A	C2-N3-C4	18.75	119.97	110.60
33	BA	519	A	C2-N3-C4	18.75	119.97	110.60
33	BA	1084	A	C2-N3-C4	18.75	119.97	110.60
33	BA	1581	A	N1-C2-N3	-18.75	119.93	129.30
33	BA	2106	A	C2-N3-C4	18.75	119.97	110.60
33	BA	2315	A	C2-N3-C4	18.75	119.97	110.60
1	AA	159	A	N1-C2-N3	-18.75	119.93	129.30
1	AA	203	A	C2-N3-C4	18.75	119.97	110.60
1	AA	696	A	C2-N3-C4	18.75	119.97	110.60
1	AA	738	A	C2-N3-C4	18.75	119.97	110.60
1	AA	975	A	N1-C2-N3	-18.75	119.93	129.30
1	AA	1031	A	C2-N3-C4	18.75	119.97	110.60
1	AA	1466	A	C2-N3-C4	18.75	119.97	110.60
33	BA	543	A	C2-N3-C4	18.75	119.97	110.60
33	BA	553	A	C2-N3-C4	18.75	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2111	A	C2-N3-C4	18.75	119.97	110.60
33	BA	2228	A	C2-N3-C4	18.75	119.97	110.60
1	AA	1207	A	C2-N3-C4	18.74	119.97	110.60
33	BA	1815	A	C2-N3-C4	18.74	119.97	110.60
1	AA	28	A	N1-C2-N3	-18.74	119.93	129.30
33	BA	224	A	N1-C2-N3	-18.74	119.93	129.30
33	BA	330	A	C2-N3-C4	18.74	119.97	110.60
33	BA	971	A	C2-N3-C4	18.74	119.97	110.60
33	BA	2080	A	C2-N3-C4	18.74	119.97	110.60
33	BA	389	A	N1-C2-N3	-18.74	119.93	129.30
33	BA	965	A	N1-C2-N3	-18.74	119.93	129.30
33	BA	1144	A	N1-C2-N3	-18.74	119.93	129.30
33	BA	1895	A	C2-N3-C4	18.74	119.97	110.60
34	BB	17	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1348	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1422	A	N1-C2-N3	-18.74	119.93	129.30
33	BA	364	A	N1-C2-N3	-18.74	119.93	129.30
33	BA	477	A	C2-N3-C4	18.74	119.97	110.60
33	BA	572	A	N1-C2-N3	-18.74	119.93	129.30
33	BA	717	A	C2-N3-C4	18.74	119.97	110.60
33	BA	786	A	C2-N3-C4	18.74	119.97	110.60
33	BA	1047	A	C2-N3-C4	18.74	119.97	110.60
33	BA	1569	A	C2-N3-C4	18.74	119.97	110.60
33	BA	2694	A	C2-N3-C4	18.74	119.97	110.60
33	BA	2846	A	C2-N3-C4	18.74	119.97	110.60
34	BB	55	A	C2-N3-C4	18.74	119.97	110.60
1	AA	556	A	N1-C2-N3	-18.74	119.93	129.30
33	BA	210	A	N1-C2-N3	-18.74	119.93	129.30
33	BA	2132	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	117	A	C2-N3-C4	18.74	119.97	110.60
1	AA	211	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	519	A	C2-N3-C4	18.74	119.97	110.60
1	AA	542	A	C2-N3-C4	18.74	119.97	110.60
1	AA	757	A	C2-N3-C4	18.74	119.97	110.60
1	AA	758	A	C2-N3-C4	18.74	119.97	110.60
1	AA	1247	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	1419	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	1493	A	C2-N3-C4	18.74	119.97	110.60
33	BA	14	A	C2-N3-C4	18.74	119.97	110.60
33	BA	84	A	C2-N3-C4	18.74	119.97	110.60
33	BA	673	A	C2-N3-C4	18.74	119.97	110.60
33	BA	1580	A	C2-N3-C4	18.74	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1620	A	C2-N3-C4	18.74	119.97	110.60
1	AA	81	A	C2-N3-C4	18.73	119.97	110.60
1	AA	679	A	C2-N3-C4	18.73	119.97	110.60
1	AA	768	A	N1-C2-N3	-18.73	119.93	129.30
1	AA	1111	A	N1-C2-N3	-18.73	119.93	129.30
1	AA	1434	A	N1-C2-N3	-18.73	119.93	129.30
33	BA	582	A	C2-N3-C4	18.73	119.97	110.60
33	BA	1533	A	N1-C2-N3	-18.73	119.93	129.30
33	BA	1942	A	C2-N3-C4	18.73	119.97	110.60
33	BA	1998	A	C2-N3-C4	18.73	119.97	110.60
33	BA	2043	A	C2-N3-C4	18.73	119.97	110.60
33	BA	2059	A	C2-N3-C4	18.73	119.97	110.60
33	BA	2078	A	C2-N3-C4	18.73	119.97	110.60
1	AA	568	A	C2-N3-C4	18.73	119.97	110.60
33	BA	38	A	C2-N3-C4	18.73	119.97	110.60
33	BA	345	A	N1-C2-N3	-18.73	119.93	129.30
33	BA	1989	A	C2-N3-C4	18.73	119.97	110.60
33	BA	2390	A	C2-N3-C4	18.73	119.97	110.60
1	AA	541	A	C2-N3-C4	18.73	119.97	110.60
1	AA	1417	A	C2-N3-C4	18.73	119.97	110.60
33	BA	162	A	C2-N3-C4	18.73	119.97	110.60
33	BA	162	A	N1-C2-N3	-18.73	119.93	129.30
33	BA	199	A	C2-N3-C4	18.73	119.97	110.60
33	BA	658	A	N1-C2-N3	-18.73	119.94	129.30
33	BA	1412	A	C2-N3-C4	18.73	119.97	110.60
33	BA	1882	A	C2-N3-C4	18.73	119.97	110.60
33	BA	2316	A	N1-C2-N3	-18.73	119.93	129.30
34	BB	76	A	C2-N3-C4	18.73	119.97	110.60
1	AA	178	A	N1-C2-N3	-18.73	119.94	129.30
1	AA	1342	A	N1-C2-N3	-18.73	119.94	129.30
33	BA	2686	A	N1-C2-N3	-18.73	119.94	129.30
1	AA	31	A	N1-C2-N3	-18.73	119.94	129.30
1	AA	118	A	C2-N3-C4	18.73	119.96	110.60
1	AA	703	A	C2-N3-C4	18.73	119.96	110.60
33	BA	244	A	N1-C2-N3	-18.73	119.94	129.30
33	BA	993	A	C2-N3-C4	18.73	119.97	110.60
33	BA	1201	A	N1-C2-N3	-18.73	119.94	129.30
33	BA	1767	A	C2-N3-C4	18.73	119.97	110.60
33	BA	1918	A	N1-C2-N3	-18.73	119.94	129.30
33	BA	1941	A	C2-N3-C4	18.73	119.96	110.60
1	AA	34	A	C2-N3-C4	18.73	119.96	110.60
1	AA	644	A	C2-N3-C4	18.73	119.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	799	A	C2-N3-C4	18.73	119.96	110.60
1	AA	1510	A	N1-C2-N3	-18.73	119.94	129.30
33	BA	437	A	N1-C2-N3	-18.73	119.94	129.30
33	BA	1947	A	C2-N3-C4	18.73	119.96	110.60
1	AA	477	A	N1-C2-N3	-18.73	119.94	129.30
1	AA	501	A	C2-N3-C4	18.73	119.96	110.60
1	AA	1077	A	N1-C2-N3	-18.73	119.94	129.30
1	AA	1225	A	C2-N3-C4	18.73	119.96	110.60
1	AA	1245	A	C2-N3-C4	18.73	119.96	110.60
1	AA	1513	A	C2-N3-C4	18.73	119.96	110.60
33	BA	740	A	C2-N3-C4	18.73	119.96	110.60
33	BA	1066	A	C2-N3-C4	18.73	119.96	110.60
33	BA	1388	A	N1-C2-N3	-18.73	119.94	129.30
33	BA	1850	A	C2-N3-C4	18.73	119.96	110.60
33	BA	2191	A	N1-C2-N3	-18.73	119.94	129.30
33	BA	2303	A	C2-N3-C4	18.73	119.96	110.60
33	BA	2455	A	C2-N3-C4	18.73	119.96	110.60
33	BA	2463	A	C2-N3-C4	18.73	119.96	110.60
33	BA	2673	A	N1-C2-N3	-18.73	119.94	129.30
34	BB	17	A	N1-C2-N3	-18.73	119.94	129.30
34	BB	43	A	C2-N3-C4	18.73	119.96	110.60
1	AA	271	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	724	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	61	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	160	A	C2-N3-C4	18.72	119.96	110.60
1	AA	232	A	C2-N3-C4	18.72	119.96	110.60
1	AA	352	A	C2-N3-C4	18.72	119.96	110.60
1	AA	460	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	704	A	C2-N3-C4	18.72	119.96	110.60
1	AA	1503	A	C2-N3-C4	18.72	119.96	110.60
33	BA	652	A	N1-C2-N3	-18.72	119.94	129.30
33	BA	1142	A	N1-C2-N3	-18.72	119.94	129.30
33	BA	1197	A	C2-N3-C4	18.72	119.96	110.60
33	BA	1339	A	C2-N3-C4	18.72	119.96	110.60
33	BA	1404	A	C2-N3-C4	18.72	119.96	110.60
33	BA	1477	A	C2-N3-C4	18.72	119.96	110.60
33	BA	1906	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	910	A	N1-C2-N3	-18.72	119.94	129.30
33	BA	41	A	C2-N3-C4	18.72	119.96	110.60
33	BA	1020	A	C2-N3-C4	18.72	119.96	110.60
33	BA	2912	A	C2-N3-C4	18.72	119.96	110.60
1	AA	1248	A	C2-N3-C4	18.72	119.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	479	A	N1-C2-N3	-18.72	119.94	129.30
33	BA	717	A	N1-C2-N3	-18.72	119.94	129.30
33	BA	1072	A	N1-C2-N3	-18.72	119.94	129.30
33	BA	1464	A	C2-N3-C4	18.72	119.96	110.60
1	AA	120	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	323	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	508	A	C2-N3-C4	18.72	119.96	110.60
1	AA	1103	A	C2-N3-C4	18.72	119.96	110.60
1	AA	287	A	C2-N3-C4	18.72	119.96	110.60
1	AA	323	A	C2-N3-C4	18.72	119.96	110.60
1	AA	367	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	618	A	C2-N3-C4	18.72	119.96	110.60
1	AA	823	A	C2-N3-C4	18.72	119.96	110.60
33	BA	421	A	N1-C2-N3	-18.72	119.94	129.30
33	BA	830	A	N1-C2-N3	-18.72	119.94	129.30
33	BA	1074	A	N1-C2-N3	-18.72	119.94	129.30
33	BA	2032	A	C2-N3-C4	18.72	119.96	110.60
34	BB	56	A	C2-N3-C4	18.72	119.96	110.60
34	BB	113	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	529	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	725	A	C2-N3-C4	18.71	119.96	110.60
1	AA	1050	A	N1-C2-N3	-18.71	119.94	129.30
33	BA	150	A	C2-N3-C4	18.71	119.96	110.60
33	BA	154	A	N1-C2-N3	-18.71	119.94	129.30
33	BA	828	A	N1-C2-N3	-18.71	119.94	129.30
33	BA	1078	A	C2-N3-C4	18.71	119.96	110.60
33	BA	1941	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	53	A	C2-N3-C4	18.71	119.96	110.60
1	AA	651	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	1006	A	C2-N3-C4	18.71	119.96	110.60
1	AA	1254	A	N1-C2-N3	-18.71	119.94	129.30
33	BA	236	A	C2-N3-C4	18.71	119.96	110.60
33	BA	561	A	C2-N3-C4	18.71	119.96	110.60
33	BA	646	A	C2-N3-C4	18.71	119.96	110.60
33	BA	828	A	C2-N3-C4	18.71	119.96	110.60
1	AA	203	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	518	A	C2-N3-C4	18.71	119.96	110.60
33	BA	438	A	N1-C2-N3	-18.71	119.94	129.30
33	BA	2619	A	C2-N3-C4	18.71	119.96	110.60
1	AA	120	A	C2-N3-C4	18.71	119.95	110.60
1	AA	604	A	C2-N3-C4	18.71	119.95	110.60
1	AA	1140	A	N1-C2-N3	-18.71	119.94	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	354	A	C2-N3-C4	18.71	119.95	110.60
33	BA	623	A	C2-N3-C4	18.71	119.95	110.60
33	BA	1202	A	N1-C2-N3	-18.71	119.94	129.30
33	BA	2071	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	568	A	N1-C2-N3	-18.71	119.95	129.30
1	AA	727	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	1270	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	1386	A	N1-C2-N3	-18.71	119.94	129.30
33	BA	1314	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	290	A	C2-N3-C4	18.71	119.95	110.60
1	AA	1102	A	N1-C2-N3	-18.71	119.95	129.30
33	BA	216	A	N1-C2-N3	-18.71	119.95	129.30
33	BA	868	A	C2-N3-C4	18.71	119.95	110.60
33	BA	958	A	C2-N3-C4	18.71	119.95	110.60
33	BA	1260	A	N1-C2-N3	-18.71	119.95	129.30
33	BA	1302	A	C2-N3-C4	18.71	119.95	110.60
33	BA	2089	A	C2-N3-C4	18.71	119.95	110.60
33	BA	2216	A	N1-C2-N3	-18.71	119.95	129.30
33	BA	2421	A	C2-N3-C4	18.71	119.95	110.60
33	BA	2762	A	N1-C2-N3	-18.71	119.95	129.30
33	BA	2845	A	N1-C2-N3	-18.71	119.95	129.30
1	AA	777	A	N1-C2-N3	-18.71	119.95	129.30
1	AA	1328	A	N1-C2-N3	-18.71	119.95	129.30
33	BA	630	A	C2-N3-C4	18.71	119.95	110.60
33	BA	1700	A	N1-C2-N3	-18.71	119.95	129.30
33	BA	2163	A	C2-N3-C4	18.71	119.95	110.60
33	BA	2455	A	N1-C2-N3	-18.71	119.95	129.30
1	AA	281	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	985	A	C2-N3-C4	18.70	119.95	110.60
1	AA	1048	A	C2-N3-C4	18.70	119.95	110.60
33	BA	206	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	917	A	C2-N3-C4	18.70	119.95	110.60
33	BA	1540	A	C2-N3-C4	18.70	119.95	110.60
33	BA	1788	A	C2-N3-C4	18.70	119.95	110.60
33	BA	1820	A	C2-N3-C4	18.70	119.95	110.60
33	BA	2851	A	N1-C2-N3	-18.70	119.95	129.30
34	BB	55	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	142	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	460	A	C2-N3-C4	18.70	119.95	110.60
1	AA	650	A	C2-N3-C4	18.70	119.95	110.60
1	AA	923	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	166	A	N1-C2-N3	-18.70	119.95	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1092	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	1119	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	1412	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	1541	A	C2-N3-C4	18.70	119.95	110.60
33	BA	1768	A	C2-N3-C4	18.70	119.95	110.60
1	AA	801	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	1259	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	1042	A	C2-N3-C4	18.70	119.95	110.60
33	BA	1517	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	2805	A	C2-N3-C4	18.70	119.95	110.60
1	AA	361	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	882	A	C2-N3-C4	18.70	119.95	110.60
1	AA	918	A	C2-N3-C4	18.70	119.95	110.60
1	AA	993	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	1056	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	1149	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	2155	A	C2-N3-C4	18.70	119.95	110.60
1	AA	1283	A	C2-N3-C4	18.70	119.95	110.60
33	BA	324	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	517	A	C2-N3-C4	18.70	119.95	110.60
33	BA	1054	A	C2-N3-C4	18.70	119.95	110.60
1	AA	672	A	C2-N3-C4	18.70	119.95	110.60
1	AA	1147	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	199	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	273	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	1393	A	C2-N3-C4	18.70	119.95	110.60
33	BA	1593	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	1727	A	C2-N3-C4	18.70	119.95	110.60
33	BA	1809	A	C2-N3-C4	18.70	119.95	110.60
33	BA	2134	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	2827	A	C2-N3-C4	18.70	119.95	110.60
33	BA	475	A	C2-N3-C4	18.70	119.95	110.60
33	BA	2658	A	N1-C2-N3	-18.70	119.95	129.30
33	BA	2778	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	52	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	232	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	382	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	456	A	N1-C2-N3	-18.69	119.95	129.30
33	BA	530	A	N1-C2-N3	-18.69	119.95	129.30
33	BA	1179	A	N1-C2-N3	-18.69	119.95	129.30
33	BA	1966	A	C2-N3-C4	18.69	119.95	110.60
33	BA	2364	A	C2-N3-C4	18.69	119.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2542	A	C2-N3-C4	18.69	119.95	110.60
33	BA	2810	A	C2-N3-C4	18.69	119.95	110.60
33	BA	1287	A	N1-C2-N3	-18.69	119.95	129.30
33	BA	1789	A	N1-C2-N3	-18.69	119.95	129.30
33	BA	2389	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	62	A	C2-N3-C4	18.69	119.94	110.60
1	AA	569	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	974	A	C2-N3-C4	18.69	119.94	110.60
1	AA	974	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	1185	A	N1-C2-N3	-18.69	119.95	129.30
33	BA	1131	A	N1-C2-N3	-18.69	119.95	129.30
33	BA	1517	A	C2-N3-C4	18.69	119.95	110.60
33	BA	2734	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	825	A	N1-C2-N3	-18.69	119.96	129.30
1	AA	1315	A	C2-N3-C4	18.69	119.94	110.60
33	BA	2593	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	757	A	N1-C2-N3	-18.69	119.96	129.30
1	AA	1443	A	C2-N3-C4	18.69	119.94	110.60
33	BA	219	A	N1-C2-N3	-18.69	119.96	129.30
33	BA	353	A	N1-C2-N3	-18.69	119.96	129.30
33	BA	762	A	N1-C2-N3	-18.69	119.96	129.30
33	BA	763	A	N1-C2-N3	-18.69	119.96	129.30
33	BA	893	A	N1-C2-N3	-18.69	119.96	129.30
33	BA	1734	A	C2-N3-C4	18.69	119.94	110.60
33	BA	1888	A	C2-N3-C4	18.69	119.94	110.60
33	BA	2923	A	N1-C2-N3	-18.69	119.96	129.30
34	BB	13	A	N1-C2-N3	-18.69	119.96	129.30
1	AA	685	A	N1-C2-N3	-18.69	119.96	129.30
1	AA	1503	A	N1-C2-N3	-18.69	119.96	129.30
33	BA	1190	A	C2-N3-C4	18.69	119.94	110.60
1	AA	209	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	569	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1197	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1266	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1296	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1297	A	C2-N3-C4	18.68	119.94	110.60
33	BA	647	A	C2-N3-C4	18.68	119.94	110.60
33	BA	1404	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	2526	A	C2-N3-C4	18.68	119.94	110.60
33	BA	2670	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1288	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	325	A	N1-C2-N3	-18.68	119.96	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	354	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1313	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1942	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	2044	A	C2-N3-C4	18.68	119.94	110.60
1	AA	128	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	189	A	C2-N3-C4	18.68	119.94	110.60
1	AA	335	A	C2-N3-C4	18.68	119.94	110.60
1	AA	344	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	496	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1048	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1077	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1213	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	13	A	C2-N3-C4	18.68	119.94	110.60
33	BA	302	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	469	A	C2-N3-C4	18.68	119.94	110.60
33	BA	974	A	C2-N3-C4	18.68	119.94	110.60
33	BA	1648	A	C2-N3-C4	18.68	119.94	110.60
33	BA	2298	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	2356	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	236	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	474	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1102	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1456	A	C2-N3-C4	18.68	119.94	110.60
33	BA	525	A	C2-N3-C4	18.68	119.94	110.60
33	BA	1130	A	C2-N3-C4	18.68	119.94	110.60
33	BA	1277	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1434	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	2315	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	2770	A	C2-N3-C4	18.68	119.94	110.60
1	AA	94	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	690	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	1161	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1528	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	584	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	867	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1066	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1339	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1499	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1815	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	2030	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	2032	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	2777	A	C2-N3-C4	18.68	119.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	228	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	240	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	537	A	C2-N3-C4	18.68	119.94	110.60
33	BA	677	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1453	A	C2-N3-C4	18.68	119.94	110.60
33	BA	1743	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1812	A	C2-N3-C4	18.68	119.94	110.60
33	BA	2454	A	C2-N3-C4	18.68	119.94	110.60
33	BA	2616	A	C2-N3-C4	18.68	119.94	110.60
34	BB	105	A	C2-N3-C4	18.68	119.94	110.60
1	AA	202	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	333	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	357	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	419	A	C2-N3-C4	18.68	119.94	110.60
1	AA	491	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	969	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1026	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	1149	A	C2-N3-C4	18.68	119.94	110.60
33	BA	1326	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	2303	A	N1-C2-N3	-18.68	119.96	129.30
33	BA	2719	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	923	A	C2-N3-C4	18.67	119.94	110.60
1	AA	947	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	1028	A	N1-C2-N3	-18.67	119.96	129.30
33	BA	727	A	C2-N3-C4	18.67	119.94	110.60
33	BA	1308	A	N1-C2-N3	-18.67	119.96	129.30
33	BA	2124	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	18	A	C2-N3-C4	18.67	119.94	110.60
1	AA	1417	A	N1-C2-N3	-18.67	119.96	129.30
33	BA	384	A	N1-C2-N3	-18.67	119.96	129.30
33	BA	1116	A	N1-C2-N3	-18.67	119.96	129.30
33	BA	1722	A	C2-N3-C4	18.67	119.94	110.60
33	BA	1791	A	C2-N3-C4	18.67	119.94	110.60
33	BA	2241	A	N1-C2-N3	-18.67	119.96	129.30
33	BA	2779	A	N1-C2-N3	-18.67	119.96	129.30
33	BA	2919	A	C2-N3-C4	18.67	119.94	110.60
1	AA	541	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	796	A	N1-C2-N3	-18.67	119.96	129.30
33	BA	202	A	C2-N3-C4	18.67	119.94	110.60
33	BA	547	A	N1-C2-N3	-18.67	119.97	129.30
33	BA	1034	A	C2-N3-C4	18.67	119.94	110.60
33	BA	1421	A	N1-C2-N3	-18.67	119.96	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1831	A	C2-N3-C4	18.67	119.94	110.60
1	AA	618	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	638	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	1294	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	1529	A	N1-C2-N3	-18.67	119.97	129.30
33	BA	2395	A	C2-N3-C4	18.67	119.94	110.60
1	AA	1248	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	1327	A	N1-C2-N3	-18.67	119.97	129.30
33	BA	339	A	C2-N3-C4	18.67	119.93	110.60
33	BA	448	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	389	A	N1-C2-N3	-18.67	119.97	129.30
33	BA	835	A	C2-N3-C4	18.67	119.93	110.60
33	BA	1677	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	296	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	831	A	C2-N3-C4	18.66	119.93	110.60
33	BA	1221	A	C2-N3-C4	18.66	119.93	110.60
33	BA	1465	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	572	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1120	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1478	A	C2-N3-C4	18.66	119.93	110.60
33	BA	1056	A	C2-N3-C4	18.66	119.93	110.60
33	BA	2083	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	189	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	485	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	684	A	C2-N3-C4	18.66	119.93	110.60
1	AA	1004	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	274	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	1175	A	C2-N3-C4	18.66	119.93	110.60
33	BA	1456	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	166	A	C2-N3-C4	18.66	119.93	110.60
33	BA	525	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	786	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	386	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	463	A	C2-N3-C4	18.66	119.93	110.60
1	AA	630	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1006	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	948	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	978	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	1188	A	C2-N3-C4	18.66	119.93	110.60
33	BA	1617	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	2060	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	2387	A	C2-N3-C4	18.66	119.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2405	A	C2-N3-C4	18.66	119.93	110.60
33	BA	2542	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	1176	A	C2-N3-C4	18.66	119.93	110.60
33	BA	53	A	C2-N3-C4	18.66	119.93	110.60
33	BA	337	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	1721	A	C2-N3-C4	18.66	119.93	110.60
33	BA	2006	A	C2-N3-C4	18.66	119.93	110.60
33	BA	2595	A	C2-N3-C4	18.66	119.93	110.60
1	AA	12	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	67	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	161	A	C2-N3-C4	18.66	119.93	110.60
33	BA	260	A	C2-N3-C4	18.66	119.93	110.60
33	BA	922	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	1075	A	C2-N3-C4	18.66	119.93	110.60
33	BA	1115	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	1175	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	1648	A	N1-C2-N3	-18.66	119.97	129.30
33	BA	1832	A	C2-N3-C4	18.66	119.93	110.60
1	AA	1479	A	N1-C2-N3	-18.65	119.97	129.30
33	BA	2405	A	N1-C2-N3	-18.65	119.97	129.30
33	BA	2787	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	190	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	1271	A	N1-C2-N3	-18.65	119.97	129.30
33	BA	73	A	N1-C2-N3	-18.65	119.97	129.30
33	BA	178	A	C2-N3-C4	18.65	119.93	110.60
33	BA	746	A	C2-N3-C4	18.65	119.93	110.60
33	BA	1025	A	N1-C2-N3	-18.65	119.97	129.30
33	BA	1253	A	C2-N3-C4	18.65	119.93	110.60
33	BA	1453	A	N1-C2-N3	-18.65	119.97	129.30
33	BA	1585	A	N1-C2-N3	-18.65	119.97	129.30
33	BA	1850	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	371	A	N1-C2-N3	-18.65	119.97	129.30
21	AX	9	A	C2-N3-C4	18.65	119.92	110.60
33	BA	752	A	C2-N3-C4	18.65	119.93	110.60
33	BA	1797	A	N1-C2-N3	-18.65	119.97	129.30
33	BA	1945	A	N1-C2-N3	-18.65	119.97	129.30
33	BA	2187	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	519	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	975	A	C2-N3-C4	18.65	119.92	110.60
33	BA	1201	A	C2-N3-C4	18.65	119.92	110.60
33	BA	1654	A	N1-C2-N3	-18.65	119.98	129.30
33	BA	2091	A	N1-C2-N3	-18.65	119.97	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	27	A	N1-C2-N3	-18.65	119.97	129.30
33	BA	436	A	N1-C2-N3	-18.65	119.98	129.30
33	BA	1360	A	N1-C2-N3	-18.65	119.98	129.30
33	BA	1432	A	C2-N3-C4	18.65	119.92	110.60
33	BA	2594	A	N1-C2-N3	-18.65	119.98	129.30
1	AA	919	A	N1-C2-N3	-18.65	119.98	129.30
1	AA	1017	A	N1-C2-N3	-18.65	119.98	129.30
1	AA	1090	A	C2-N3-C4	18.65	119.92	110.60
33	BA	1014	A	N1-C2-N3	-18.65	119.98	129.30
33	BA	1244	A	N1-C2-N3	-18.65	119.98	129.30
33	BA	1312	A	N1-C2-N3	-18.65	119.98	129.30
33	BA	1967	A	N1-C2-N3	-18.65	119.98	129.30
1	AA	401	A	C2-N3-C4	18.64	119.92	110.60
1	AA	1143	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	866	A	C2-N3-C4	18.64	119.92	110.60
33	BA	2860	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	824	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	969	A	C2-N3-C4	18.64	119.92	110.60
33	BA	90	A	C2-N3-C4	18.64	119.92	110.60
33	BA	110	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	758	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	829	A	C2-N3-C4	18.64	119.92	110.60
33	BA	1406	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	2364	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	2440	A	C2-N3-C4	18.64	119.92	110.60
1	AA	532	A	C2-N3-C4	18.64	119.92	110.60
1	AA	929	A	C2-N3-C4	18.64	119.92	110.60
1	AA	1366	A	C2-N3-C4	18.64	119.92	110.60
33	BA	2601	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	314	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	583	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1512	A	C2-N3-C4	18.64	119.92	110.60
33	BA	247	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	559	A	C2-N3-C4	18.64	119.92	110.60
33	BA	1161	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	2000	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	2170	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	2390	A	N1-C2-N3	-18.64	119.98	129.30
34	BB	97	A	C2-N3-C4	18.64	119.92	110.60
33	BA	229	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	355	A	C2-N3-C4	18.64	119.92	110.60
33	BA	1230	A	N1-C2-N3	-18.64	119.98	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2570	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	2770	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	290	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	532	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	851	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	1553	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	786	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1257	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	1375	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	2307	A	N1-C2-N3	-18.64	119.98	129.30
33	BA	2875	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	979	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	1509	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	500	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	390	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	582	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	1403	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	220	A	C2-N3-C4	18.63	119.92	110.60
33	BA	1948	A	C2-N3-C4	18.63	119.92	110.60
33	BA	2782	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	2904	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	987	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	653	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	1929	A	C2-N3-C4	18.63	119.92	110.60
1	AA	35	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	1328	A	C2-N3-C4	18.63	119.92	110.60
1	AA	1541	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	194	A	C2-N3-C4	18.63	119.92	110.60
33	BA	538	A	C2-N3-C4	18.63	119.92	110.60
33	BA	1113	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	1542	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	1663	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	1901	A	C2-N3-C4	18.63	119.92	110.60
33	BA	2296	A	C2-N3-C4	18.63	119.92	110.60
33	BA	2417	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	2571	A	N1-C2-N3	-18.63	119.98	129.30
33	BA	2668	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	423	A	N1-C2-N3	-18.63	119.99	129.30
1	AA	53	A	N1-C2-N3	-18.63	119.99	129.30
1	AA	1296	A	N1-C2-N3	-18.63	119.99	129.30
33	BA	1073	A	N1-C2-N3	-18.63	119.99	129.30
33	BA	1174	A	N1-C2-N3	-18.63	119.99	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1724	A	C2-N3-C4	18.63	119.91	110.60
33	BA	2062	A	C2-N3-C4	18.63	119.91	110.60
33	BA	388	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	1929	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	658	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	823	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1210	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	943	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	2155	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	2317	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	2643	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	210	A	C2-N3-C4	18.62	119.91	110.60
33	BA	2869	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	504	A	C2-N3-C4	18.62	119.91	110.60
1	AA	790	A	C2-N3-C4	18.62	119.91	110.60
1	AA	816	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1236	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1294	A	C2-N3-C4	18.62	119.91	110.60
1	AA	1333	A	C2-N3-C4	18.62	119.91	110.60
33	BA	5	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	1966	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	1981	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	258	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	616	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	705	A	C2-N3-C4	18.62	119.91	110.60
33	BA	1583	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	2338	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	308	A	C2-N3-C4	18.62	119.91	110.60
1	AA	870	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	176	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	202	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	373	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	1323	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	1361	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	1464	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	1746	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	1802	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	1238	A	C2-N3-C4	18.62	119.91	110.60
33	BA	582	A	N1-C2-N3	-18.62	119.99	129.30
33	BA	2769	A	N1-C2-N3	-18.62	119.99	129.30
1	AA	684	A	N1-C2-N3	-18.61	119.99	129.30
33	BA	2152	A	N1-C2-N3	-18.61	119.99	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2441	A	C2-N3-C4	18.61	119.91	110.60
34	BB	51	A	N1-C2-N3	-18.61	119.99	129.30
1	AA	883	A	C2-N3-C4	18.61	119.91	110.60
33	BA	343	A	C2-N3-C4	18.61	119.91	110.60
33	BA	917	A	N1-C2-N3	-18.61	119.99	129.30
33	BA	1735	A	N1-C2-N3	-18.61	119.99	129.30
1	AA	439	A	N1-C2-N3	-18.61	120.00	129.30
33	BA	678	A	C2-N3-C4	18.61	119.91	110.60
33	BA	1504	A	N1-C2-N3	-18.61	120.00	129.30
33	BA	1760	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	1128	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	1407	A	C2-N3-C4	18.61	119.90	110.60
33	BA	117	A	C2-N3-C4	18.61	119.90	110.60
33	BA	518	A	C2-N3-C4	18.61	119.90	110.60
33	BA	1592	A	N1-C2-N3	-18.61	120.00	129.30
33	BA	1685	A	N1-C2-N3	-18.61	120.00	129.30
33	BA	2141	A	N1-C2-N3	-18.61	120.00	129.30
33	BA	2256	A	N1-C2-N3	-18.61	120.00	129.30
33	BA	2526	A	N1-C2-N3	-18.61	120.00	129.30
33	BA	637	A	N1-C2-N3	-18.61	120.00	129.30
33	BA	876	A	N1-C2-N3	-18.61	120.00	129.30
1	AA	266	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	462	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	583	A	C2-N3-C4	18.60	119.90	110.60
33	BA	222	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	254	A	C2-N3-C4	18.60	119.90	110.60
33	BA	1423	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	2007	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	2826	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	964	A	C2-N3-C4	18.60	119.90	110.60
33	BA	1679	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	1115	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	65	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	490	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	553	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	1767	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	2339	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	1031	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	1502	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	322	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	1536	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	1606	A	C2-N3-C4	18.60	119.90	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	160	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	352	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	268	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	904	A	C2-N3-C4	18.60	119.90	110.60
33	BA	1627	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	2498	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	2740	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	124	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	1254	A	N1-C2-N3	-18.60	120.00	129.30
33	BA	1619	A	C2-N3-C4	18.60	119.90	110.60
1	AA	173	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	828	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	1588	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	1818	A	C2-N3-C4	18.59	119.90	110.60
33	BA	1982	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	808	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	1224	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	2087	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	251	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	372	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	679	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	868	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	1021	A	C2-N3-C4	18.59	119.90	110.60
33	BA	1084	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	1995	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	2047	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	2691	A	C2-N3-C4	18.59	119.90	110.60
33	BA	2835	A	C2-N3-C4	18.59	119.90	110.60
1	AA	548	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	1121	A	N1-C2-N3	-18.59	120.00	129.30
21	AX	58	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	519	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	782	A	N1-C2-N3	-18.59	120.00	129.30
34	BB	64	A	N1-C2-N3	-18.59	120.00	129.30
34	BB	114	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	129	A	N1-C2-N3	-18.59	120.01	129.30
1	AA	650	A	N1-C2-N3	-18.59	120.01	129.30
1	AA	1222	A	N1-C2-N3	-18.59	120.01	129.30
1	AA	1451	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	225	A	N1-C2-N3	-18.59	120.00	129.30
33	BA	231	A	N1-C2-N3	-18.59	120.01	129.30
33	BA	2042	A	N1-C2-N3	-18.59	120.00	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2165	A	N1-C2-N3	-18.59	120.01	129.30
33	BA	2421	A	N1-C2-N3	-18.59	120.01	129.30
33	BA	2461	A	N1-C2-N3	-18.59	120.00	129.30
34	BB	43	A	N1-C2-N3	-18.59	120.01	129.30
1	AA	1384	A	C2-N3-C4	18.59	119.89	110.60
33	BA	1335	A	N1-C2-N3	-18.59	120.01	129.30
33	BA	1516	A	N1-C2-N3	-18.59	120.01	129.30
33	BA	94	A	N1-C2-N3	-18.59	120.01	129.30
33	BA	888	A	N1-C2-N3	-18.59	120.01	129.30
33	BA	1027	A	N1-C2-N3	-18.59	120.01	129.30
33	BA	1094	A	C2-N3-C4	18.59	119.89	110.60
33	BA	1722	A	N1-C2-N3	-18.59	120.01	129.30
34	BB	20	A	N1-C2-N3	-18.59	120.01	129.30
33	BA	459	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	661	A	C2-N3-C4	18.58	119.89	110.60
1	AA	459	A	N1-C2-N3	-18.58	120.01	129.30
21	AX	76	A	C2-N3-C4	18.58	119.89	110.60
33	BA	91	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	524	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	811	A	C2-N3-C4	18.58	119.89	110.60
33	BA	1034	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	2252	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	2511	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	555	A	N1-C2-N3	-18.58	120.01	129.30
21	AX	21	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	150	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	200	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	329	A	C2-N3-C4	18.58	119.89	110.60
1	AA	959	A	C2-N3-C4	18.58	119.89	110.60
1	AA	1513	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	333	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	1723	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	1913	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	2381	A	C2-N3-C4	18.58	119.89	110.60
1	AA	978	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	61	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	84	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	727	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	908	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	2187	A	C2-N3-C4	18.58	119.89	110.60
33	BA	2595	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	2704	A	N1-C2-N3	-18.58	120.01	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	669	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	1225	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	193	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	339	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	835	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	1078	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	2661	A	N1-C2-N3	-18.58	120.01	129.30
33	BA	2750	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	671	A	N1-C2-N3	-18.57	120.01	129.30
33	BA	412	A	N1-C2-N3	-18.57	120.01	129.30
33	BA	699	A	N1-C2-N3	-18.57	120.01	129.30
33	BA	722	A	C2-N3-C4	18.57	119.89	110.60
33	BA	947	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	762	A	N1-C2-N3	-18.57	120.01	129.30
1	AA	1422	A	C2-N3-C4	18.57	119.89	110.60
33	BA	1608	A	N1-C2-N3	-18.57	120.01	129.30
33	BA	2606	A	C2-N3-C4	18.57	119.89	110.60
1	AA	475	A	N1-C2-N3	-18.57	120.01	129.30
33	BA	470	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	646	A	N1-C2-N3	-18.57	120.01	129.30
33	BA	1848	A	N1-C2-N3	-18.57	120.01	129.30
33	BA	2164	A	C2-N3-C4	18.57	119.89	110.60
33	BA	2383	A	C2-N3-C4	18.57	119.89	110.60
1	AA	1103	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	1189	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	548	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	1791	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	2907	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	1466	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	258	A	C2-N3-C4	18.57	119.88	110.60
33	BA	1019	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	1134	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	1876	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	1176	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	139	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	522	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	1180	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	102	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	543	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	600	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	746	A	N1-C2-N3	-18.57	120.02	129.30
33	BA	1020	A	N1-C2-N3	-18.57	120.02	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	803	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	2834	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	204	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	225	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	581	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	611	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	198	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	428	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	1006	A	C2-N3-C4	18.56	119.88	110.60
33	BA	1699	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	1883	A	C2-N3-C4	18.56	119.88	110.60
33	BA	2227	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	2468	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	2887	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	117	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	781	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	1534	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	1556	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	62	A	N1-C2-N3	-18.56	120.02	129.30
21	AX	41	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	917	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	1014	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	753	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	210	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	1221	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	1265	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	1631	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	1721	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	1809	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	1901	A	N1-C2-N3	-18.56	120.02	129.30
33	BA	376	A	N1-C2-N3	-18.55	120.02	129.30
33	BA	1291	A	C2-N3-C4	18.55	119.88	110.60
33	BA	2340	A	C2-N3-C4	18.55	119.88	110.60
1	AA	415	A	C2-N3-C4	18.55	119.88	110.60
1	AA	862	A	C2-N3-C4	18.55	119.88	110.60
1	AA	1442	A	N1-C2-N3	-18.55	120.02	129.30
33	BA	1928	A	N1-C2-N3	-18.55	120.02	129.30
33	BA	2912	A	N1-C2-N3	-18.55	120.02	129.30
34	BB	56	A	N1-C2-N3	-18.55	120.02	129.30
1	AA	118	A	N1-C2-N3	-18.55	120.02	129.30
33	BA	355	A	N1-C2-N3	-18.55	120.02	129.30
33	BA	429	A	N1-C2-N3	-18.55	120.02	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	904	A	N1-C2-N3	-18.55	120.02	129.30
33	BA	958	A	N1-C2-N3	-18.55	120.02	129.30
33	BA	1745	A	C2-N3-C4	18.55	119.88	110.60
33	BA	1885	A	N1-C2-N3	-18.55	120.02	129.30
33	BA	1381	A	N1-C2-N3	-18.55	120.03	129.30
33	BA	2148	A	N1-C2-N3	-18.55	120.02	129.30
33	BA	179	A	C2-N3-C4	18.55	119.88	110.60
33	BA	1788	A	N1-C2-N3	-18.55	120.03	129.30
33	BA	1620	A	N1-C2-N3	-18.55	120.03	129.30
33	BA	1838	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	886	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	902	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	1161	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	1359	A	N1-C2-N3	-18.55	120.03	129.30
33	BA	6	A	N1-C2-N3	-18.55	120.03	129.30
33	BA	236	A	N1-C2-N3	-18.55	120.03	129.30
33	BA	1130	A	N1-C2-N3	-18.55	120.03	129.30
33	BA	1445	A	N1-C2-N3	-18.55	120.03	129.30
33	BA	1900	A	N1-C2-N3	-18.55	120.03	129.30
33	BA	2049	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	696	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	21	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	705	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	1405	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	1839	A	C2-N3-C4	18.54	119.87	110.60
1	AA	107	A	C2-N3-C4	18.54	119.87	110.60
1	AA	811	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1054	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	2505	A	N1-C2-N3	-18.54	120.03	129.30
34	BB	50	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	592	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	2407	A	C2-N3-C4	18.54	119.87	110.60
1	AA	1092	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1252	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	2241	A	C2-N3-C4	18.54	119.87	110.60
33	BA	2902	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	799	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	574	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	689	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	1346	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	1461	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	1532	A	N1-C2-N3	-18.54	120.03	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2330	A	C2-N3-C4	18.54	119.87	110.60
1	AA	452	A	N1-C2-N3	-18.54	120.03	129.30
33	BA	1774	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	911	A	C2-N3-C4	18.53	119.87	110.60
33	BA	318	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	449	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	1055	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	1243	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	1575	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	1686	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	1697	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	1054	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	1734	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	14	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	1520	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	2146	A	N1-C2-N3	-18.53	120.03	129.30
1	AA	1197	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	13	A	N1-C2-N3	-18.53	120.03	129.30
33	BA	52	A	C2-N3-C4	18.53	119.86	110.60
33	BA	168	A	C2-N3-C4	18.53	119.86	110.60
33	BA	692	A	N1-C2-N3	-18.53	120.03	129.30
1	AA	738	A	N1-C2-N3	-18.53	120.04	129.30
33	BA	10	A	N1-C2-N3	-18.53	120.04	129.30
33	BA	259	A	N1-C2-N3	-18.53	120.04	129.30
33	BA	1812	A	N1-C2-N3	-18.53	120.04	129.30
33	BA	2297	A	C2-N3-C4	18.53	119.86	110.60
1	AA	644	A	N1-C2-N3	-18.53	120.04	129.30
1	AA	1383	A	N1-C2-N3	-18.53	120.04	129.30
33	BA	2078	A	N1-C2-N3	-18.53	120.04	129.30
1	AA	287	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	307	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	2387	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	2463	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	2477	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	1523	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	126	A	C2-N3-C4	18.52	119.86	110.60
1	AA	677	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	879	A	C2-N3-C4	18.52	119.86	110.60
33	BA	507	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	1056	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	2406	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	67	A	C2-N3-C4	18.52	119.86	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1233	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	1948	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	2327	A	N1-C2-N3	-18.52	120.04	129.30
33	BA	2805	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	659	A	N1-C2-N3	-18.51	120.04	129.30
1	AA	984	A	N1-C2-N3	-18.51	120.04	129.30
33	BA	952	A	N1-C2-N3	-18.51	120.04	129.30
33	BA	1540	A	N1-C2-N3	-18.51	120.04	129.30
33	BA	1845	A	N1-C2-N3	-18.51	120.04	129.30
33	BA	2804	A	C2-N3-C4	18.51	119.86	110.60
33	BA	537	A	N1-C2-N3	-18.51	120.04	129.30
33	BA	2357	A	N1-C2-N3	-18.51	120.04	129.30
1	AA	704	A	N1-C2-N3	-18.51	120.05	129.30
1	AA	1022	A	N1-C2-N3	-18.51	120.05	129.30
33	BA	993	A	N1-C2-N3	-18.51	120.05	129.30
33	BA	2462	A	N1-C2-N3	-18.51	120.05	129.30
1	AA	1188	A	N1-C2-N3	-18.51	120.05	129.30
1	AA	1284	A	N1-C2-N3	-18.51	120.05	129.30
1	AA	1297	A	N1-C2-N3	-18.51	120.05	129.30
33	BA	2119	A	N1-C2-N3	-18.51	120.05	129.30
33	BA	2560	A	N1-C2-N3	-18.51	120.05	129.30
1	AA	1278	A	C2-N3-C4	18.50	119.85	110.60
33	BA	144	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	281	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	1606	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	1989	A	N1-C2-N3	-18.50	120.05	129.30
34	BB	18	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	2383	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	894	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	1047	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	2464	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	209	A	C2-N3-C4	18.50	119.85	110.60
1	AA	335	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	431	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	490	A	C2-N3-C4	18.50	119.85	110.60
33	BA	882	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	1483	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	1615	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	2365	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	2786	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	2827	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	2885	A	C2-N3-C4	18.50	119.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1895	A	N1-C2-N3	-18.50	120.05	129.30
34	BB	37	A	C2-N3-C4	18.50	119.85	110.60
33	BA	987	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	1569	A	N1-C2-N3	-18.50	120.05	129.30
33	BA	1925	A	N1-C2-N3	-18.50	120.05	129.30
34	BB	76	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	831	A	N1-C2-N3	-18.49	120.05	129.30
33	BA	140	A	N1-C2-N3	-18.49	120.05	129.30
33	BA	2034	A	N1-C2-N3	-18.49	120.05	129.30
33	BA	2835	A	N1-C2-N3	-18.49	120.05	129.30
1	AA	1155	A	N1-C2-N3	-18.49	120.05	129.30
33	BA	1709	A	N1-C2-N3	-18.49	120.05	129.30
33	BA	326	A	N1-C2-N3	-18.49	120.05	129.30
33	BA	2447	A	N1-C2-N3	-18.49	120.05	129.30
1	AA	1493	A	N1-C2-N3	-18.49	120.06	129.30
21	AX	44	A	N1-C2-N3	-18.49	120.06	129.30
33	BA	260	A	N1-C2-N3	-18.49	120.06	129.30
33	BA	1210	A	N1-C2-N3	-18.49	120.06	129.30
33	BA	1655	A	N1-C2-N3	-18.49	120.06	129.30
33	BA	2381	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	114	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	1179	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	1437	A	N1-C2-N3	-18.49	120.06	129.30
33	BA	125	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	391	A	C2-N3-C4	18.49	119.84	110.60
1	AA	929	A	N1-C2-N3	-18.49	120.06	129.30
33	BA	230	A	N1-C2-N3	-18.49	120.06	129.30
33	BA	1284	A	N1-C2-N3	-18.49	120.06	129.30
33	BA	2302	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	76	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	275	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	578	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	81	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	2629	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	1206	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	870	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	1965	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	2228	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	2454	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	2601	A	C2-N3-C4	18.48	119.84	110.60
33	BA	2754	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	2794	A	N1-C2-N3	-18.48	120.06	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	496	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	971	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	279	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	630	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	183	A	C2-N3-C4	18.48	119.84	110.60
33	BA	1580	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	1614	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	2830	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	161	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	1024	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	1026	A	C2-N3-C4	18.48	119.84	110.60
1	AA	1463	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	1675	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	1947	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	2900	A	N1-C2-N3	-18.48	120.06	129.30
33	BA	517	A	N1-C2-N3	-18.47	120.06	129.30
33	BA	679	A	C2-N3-C4	18.47	119.84	110.60
33	BA	1961	A	N1-C2-N3	-18.47	120.06	129.30
1	AA	604	A	N1-C2-N3	-18.47	120.06	129.30
33	BA	1768	A	N1-C2-N3	-18.47	120.06	129.30
1	AA	956	A	N1-C2-N3	-18.47	120.06	129.30
33	BA	12	A	N1-C2-N3	-18.47	120.06	129.30
33	BA	740	A	N1-C2-N3	-18.47	120.07	129.30
1	AA	1456	A	N1-C2-N3	-18.47	120.07	129.30
33	BA	278	A	N1-C2-N3	-18.47	120.07	129.30
33	BA	1003	A	N1-C2-N3	-18.47	120.07	129.30
33	BA	1424	A	N1-C2-N3	-18.47	120.07	129.30
33	BA	1680	A	N1-C2-N3	-18.47	120.07	129.30
33	BA	2497	A	N1-C2-N3	-18.47	120.07	129.30
21	AX	23	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	2066	A	N1-C2-N3	-18.46	120.07	129.30
1	AA	329	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	561	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	616	A	N1-C2-N3	-18.46	120.07	129.30
1	AA	705	A	N1-C2-N3	-18.46	120.07	129.30
1	AA	1065	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	369	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	829	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	1667	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	1882	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	1197	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	770	A	N1-C2-N3	-18.46	120.07	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1477	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	2627	A	C2-N3-C4	18.46	119.83	110.60
33	BA	2722	A	N1-C2-N3	-18.46	120.07	129.30
34	BB	105	A	N1-C2-N3	-18.46	120.07	129.30
1	AA	1425	A	N1-C2-N3	-18.46	120.07	129.30
33	BA	1877	A	N1-C2-N3	-18.46	120.07	129.30
1	AA	504	A	N1-C2-N3	-18.45	120.07	129.30
33	BA	549	A	N1-C2-N3	-18.45	120.07	129.30
33	BA	1998	A	N1-C2-N3	-18.45	120.07	129.30
33	BA	2663	A	N1-C2-N3	-18.45	120.07	129.30
1	AA	1405	A	N1-C2-N3	-18.45	120.07	129.30
33	BA	2837	A	N1-C2-N3	-18.45	120.07	129.30
1	AA	793	A	N1-C2-N3	-18.45	120.07	129.30
1	AA	1435	A	N1-C2-N3	-18.45	120.08	129.30
33	BA	343	A	N1-C2-N3	-18.45	120.07	129.30
33	BA	769	A	N1-C2-N3	-18.45	120.08	129.30
33	BA	329	A	N1-C2-N3	-18.45	120.08	129.30
33	BA	1618	A	C2-N3-C4	18.45	119.82	110.60
1	AA	234	A	N1-C2-N3	-18.45	120.08	129.30
1	AA	874	A	N1-C2-N3	-18.45	120.08	129.30
1	AA	1348	A	N1-C2-N3	-18.45	120.08	129.30
33	BA	1818	A	N1-C2-N3	-18.45	120.08	129.30
33	BA	133	A	N1-C2-N3	-18.44	120.08	129.30
33	BA	117	A	N1-C2-N3	-18.44	120.08	129.30
33	BA	1059	A	N1-C2-N3	-18.44	120.08	129.30
33	BA	1194	A	N1-C2-N3	-18.44	120.08	129.30
33	BA	2080	A	N1-C2-N3	-18.44	120.08	129.30
1	AA	1341	A	N1-C2-N3	-18.44	120.08	129.30
33	BA	964	A	N1-C2-N3	-18.44	120.08	129.30
1	AA	34	A	N1-C2-N3	-18.44	120.08	129.30
1	AA	928	A	N1-C2-N3	-18.44	120.08	129.30
33	BA	53	A	N1-C2-N3	-18.44	120.08	129.30
33	BA	173	A	N1-C2-N3	-18.44	120.08	129.30
33	BA	1957	A	C2-N3-C4	18.44	119.82	110.60
33	BA	1008	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	404	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	875	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	996	A	N1-C2-N3	-18.43	120.08	129.30
33	BA	2694	A	N1-C2-N3	-18.43	120.08	129.30
33	BA	2700	A	N1-C2-N3	-18.43	120.08	129.30
33	BA	2846	A	N1-C2-N3	-18.43	120.08	129.30
33	BA	2889	A	N1-C2-N3	-18.43	120.08	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2369	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	463	A	N1-C2-N3	-18.43	120.09	129.30
33	BA	330	A	N1-C2-N3	-18.43	120.09	129.30
33	BA	1541	A	N1-C2-N3	-18.43	120.09	129.30
33	BA	2349	A	N1-C2-N3	-18.43	120.09	129.30
33	BA	501	A	N1-C2-N3	-18.42	120.09	129.30
33	BA	622	A	N1-C2-N3	-18.42	120.09	129.30
33	BA	2006	A	N1-C2-N3	-18.42	120.09	129.30
1	AA	1366	A	N1-C2-N3	-18.42	120.09	129.30
33	BA	1126	A	N1-C2-N3	-18.42	120.09	129.30
33	BA	2441	A	N1-C2-N3	-18.42	120.09	129.30
1	AA	278	A	N1-C2-N3	-18.42	120.09	129.30
1	AA	664	A	N1-C2-N3	-18.42	120.09	129.30
33	BA	1727	A	N1-C2-N3	-18.42	120.09	129.30
33	BA	2202	A	N1-C2-N3	-18.42	120.09	129.30
33	BA	171	A	N1-C2-N3	-18.41	120.09	129.30
1	AA	918	A	N1-C2-N3	-18.41	120.09	129.30
33	BA	811	A	N1-C2-N3	-18.41	120.09	129.30
33	BA	1291	A	N1-C2-N3	-18.41	120.09	129.30
33	BA	2200	A	N1-C2-N3	-18.41	120.09	129.30
33	BA	790	A	N1-C2-N3	-18.41	120.09	129.30
33	BA	913	A	N1-C2-N3	-18.41	120.09	129.30
33	BA	462	A	N1-C2-N3	-18.41	120.09	129.30
33	BA	1888	A	N1-C2-N3	-18.41	120.09	129.30
33	BA	2854	A	N1-C2-N3	-18.41	120.09	129.30
33	BA	2924	A	N1-C2-N3	-18.41	120.09	129.30
33	BA	722	A	N1-C2-N3	-18.41	120.10	129.30
33	BA	1636	A	N1-C2-N3	-18.41	120.10	129.30
33	BA	1695	A	N1-C2-N3	-18.41	120.10	129.30
33	BA	41	A	N1-C2-N3	-18.41	120.10	129.30
1	AA	1245	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	1349	A	N1-C2-N3	-18.40	120.10	129.30
33	BA	1831	A	N1-C2-N3	-18.40	120.10	129.30
34	BB	37	A	N1-C2-N3	-18.40	120.10	129.30
33	BA	194	A	N1-C2-N3	-18.40	120.10	129.30
33	BA	2143	A	N1-C2-N3	-18.40	120.10	129.30
33	BA	1003	A	C2-N3-C4	18.40	119.80	110.60
33	BA	1724	A	N1-C2-N3	-18.40	120.10	129.30
33	BA	2052	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	72	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	270	A	N1-C2-N3	-18.40	120.10	129.30
1	AA	1443	A	N1-C2-N3	-18.40	120.10	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1392	A	N1-C2-N3	-18.40	120.10	129.30
33	BA	2297	A	N1-C2-N3	-18.40	120.10	129.30
33	BA	2689	A	N1-C2-N3	-18.39	120.10	129.30
1	AA	1283	A	N1-C2-N3	-18.39	120.10	129.30
33	BA	486	A	N1-C2-N3	-18.39	120.10	129.30
33	BA	513	A	C2-N3-C4	18.39	119.80	110.60
1	AA	988	A	C2-N3-C4	18.39	119.80	110.60
1	AA	346	A	N1-C2-N3	-18.39	120.11	129.30
1	AA	883	A	N1-C2-N3	-18.39	120.10	129.30
1	AA	771	A	N1-C2-N3	-18.39	120.11	129.30
33	BA	90	A	N1-C2-N3	-18.39	120.11	129.30
33	BA	2176	A	N1-C2-N3	-18.39	120.11	129.30
1	AA	1016	A	N1-C2-N3	-18.39	120.11	129.30
33	BA	220	A	N1-C2-N3	-18.39	120.11	129.30
33	BA	2440	A	N1-C2-N3	-18.39	120.11	129.30
1	AA	301	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	512	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	617	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	1486	A	N1-C2-N3	-18.38	120.11	129.30
33	BA	623	A	N1-C2-N3	-18.38	120.11	129.30
33	BA	667	A	C2-N3-C4	18.38	119.79	110.60
1	AA	913	A	N1-C2-N3	-18.38	120.11	129.30
33	BA	673	A	N1-C2-N3	-18.38	120.11	129.30
33	BA	724	A	N1-C2-N3	-18.38	120.11	129.30
33	BA	1672	A	N1-C2-N3	-18.38	120.11	129.30
33	BA	1999	A	N1-C2-N3	-18.38	120.11	129.30
34	BB	97	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	57	A	N1-C2-N3	-18.38	120.11	129.30
33	BA	2662	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	55	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	672	A	N1-C2-N3	-18.38	120.11	129.30
33	BA	67	A	N1-C2-N3	-18.37	120.11	129.30
33	BA	2026	A	N1-C2-N3	-18.37	120.11	129.30
33	BA	2044	A	N1-C2-N3	-18.37	120.11	129.30
33	BA	2351	A	N1-C2-N3	-18.37	120.11	129.30
33	BA	179	A	N1-C2-N3	-18.37	120.11	129.30
33	BA	2296	A	N1-C2-N3	-18.37	120.11	129.30
1	AA	1517	A	N1-C2-N3	-18.37	120.11	129.30
33	BA	2831	A	N1-C2-N3	-18.37	120.12	129.30
33	BA	538	A	N1-C2-N3	-18.37	120.12	129.30
33	BA	2343	A	N1-C2-N3	-18.37	120.12	129.30
1	AA	518	A	N1-C2-N3	-18.37	120.12	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	390	A	N1-C2-N3	-18.37	120.12	129.30
33	BA	391	A	N1-C2-N3	-18.37	120.12	129.30
33	BA	2616	A	N1-C2-N3	-18.36	120.12	129.30
1	AA	1490	A	N1-C2-N3	-18.36	120.12	129.30
33	BA	1021	A	N1-C2-N3	-18.36	120.12	129.30
33	BA	1524	A	N1-C2-N3	-18.36	120.12	129.30
33	BA	2340	A	N1-C2-N3	-18.36	120.12	129.30
33	BA	1562	A	N1-C2-N3	-18.36	120.12	129.30
1	AA	882	A	N1-C2-N3	-18.35	120.12	129.30
33	BA	156	A	N1-C2-N3	-18.35	120.12	129.30
1	AA	74	A	N1-C2-N3	-18.35	120.12	129.30
1	AA	107	A	N1-C2-N3	-18.35	120.12	129.30
1	AA	1320	A	N1-C2-N3	-18.35	120.12	129.30
33	BA	956	A	N1-C2-N3	-18.35	120.12	129.30
1	AA	337	A	N1-C2-N3	-18.35	120.13	129.30
33	BA	2395	A	N1-C2-N3	-18.35	120.13	129.30
33	BA	456	A	N1-C2-N3	-18.35	120.13	129.30
33	BA	889	A	N1-C2-N3	-18.35	120.13	129.30
1	AA	1478	A	N1-C2-N3	-18.34	120.13	129.30
33	BA	1485	A	N1-C2-N3	-18.34	120.13	129.30
1	AA	1427	A	N1-C2-N3	-18.34	120.13	129.30
33	BA	1619	A	N1-C2-N3	-18.34	120.13	129.30
33	BA	44	A	N1-C2-N3	-18.34	120.13	129.30
1	AA	711	A	N1-C2-N3	-18.34	120.13	129.30
33	BA	1100	A	N1-C2-N3	-18.34	120.13	129.30
33	BA	1832	A	N1-C2-N3	-18.33	120.13	129.30
33	BA	1096	A	N1-C2-N3	-18.33	120.13	129.30
33	BA	1235	A	N1-C2-N3	-18.33	120.13	129.30
33	BA	1956	A	N1-C2-N3	-18.33	120.13	129.30
33	BA	661	A	N1-C2-N3	-18.33	120.13	129.30
33	BA	752	A	N1-C2-N3	-18.33	120.14	129.30
1	AA	725	A	N1-C2-N3	-18.33	120.14	129.30
21	AX	76	A	N1-C2-N3	-18.33	120.14	129.30
33	BA	1286	A	N1-C2-N3	-18.33	120.14	129.30
33	BA	1982	A	C2-N3-C4	18.33	119.77	110.60
33	BA	1426	A	N1-C2-N3	-18.33	120.14	129.30
33	BA	1820	A	N1-C2-N3	-18.33	120.14	129.30
33	BA	2919	A	N1-C2-N3	-18.33	120.14	129.30
33	BA	1253	A	N1-C2-N3	-18.32	120.14	129.30
33	BA	1258	A	N1-C2-N3	-18.32	120.14	129.30
1	AA	433	A	N1-C2-N3	-18.32	120.14	129.30
33	BA	2164	A	N1-C2-N3	-18.32	120.14	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	743	A	N1-C2-N3	-18.32	120.14	129.30
33	BA	1957	A	N1-C2-N3	-18.32	120.14	129.30
33	BA	469	A	N1-C2-N3	-18.31	120.14	129.30
1	AA	282	A	N1-C2-N3	-18.31	120.14	129.30
33	BA	1393	A	N1-C2-N3	-18.31	120.14	129.30
33	BA	1222	A	N1-C2-N3	-18.31	120.15	129.30
33	BA	2790	A	N1-C2-N3	-18.31	120.14	129.30
33	BA	2500	A	N1-C2-N3	-18.31	120.15	129.30
1	AA	1384	A	N1-C2-N3	-18.31	120.15	129.30
33	BA	2100	A	N1-C2-N3	-18.31	120.15	129.30
21	AX	70	A	N1-C2-N3	-18.30	120.15	129.30
33	BA	1776	A	N1-C2-N3	-18.30	120.15	129.30
33	BA	2804	A	N1-C2-N3	-18.30	120.15	129.30
33	BA	2043	A	N1-C2-N3	-18.30	120.15	129.30
33	BA	970	A	N1-C2-N3	-18.30	120.15	129.30
1	AA	140	A	N1-C2-N3	-18.30	120.15	129.30
1	AA	397	A	N1-C2-N3	-18.30	120.15	129.30
1	AA	721	A	N1-C2-N3	-18.30	120.15	129.30
33	BA	2590	A	N1-C2-N3	-18.30	120.15	129.30
33	BA	2619	A	N1-C2-N3	-18.30	120.15	129.30
33	BA	2111	A	N1-C2-N3	-18.29	120.15	129.30
1	AA	1272	A	N1-C2-N3	-18.29	120.16	129.30
33	BA	407	A	N1-C2-N3	-18.29	120.16	129.30
33	BA	1075	A	N1-C2-N3	-18.29	120.16	129.30
33	BA	130	A	N1-C2-N3	-18.28	120.16	129.30
1	AA	1333	A	N1-C2-N3	-18.28	120.16	129.30
33	BA	2270	A	N1-C2-N3	-18.28	120.16	129.30
33	BA	518	A	N1-C2-N3	-18.27	120.16	129.30
33	BA	1094	A	N1-C2-N3	-18.27	120.16	129.30
33	BA	2459	A	N1-C2-N3	-18.27	120.16	129.30
33	BA	2517	A	N1-C2-N3	-18.27	120.17	129.30
33	BA	896	A	N1-C2-N3	-18.27	120.17	129.30
33	BA	1653	A	N1-C2-N3	-18.27	120.17	129.30
1	AA	605	A	N1-C2-N3	-18.27	120.17	129.30
33	BA	1357	A	N1-C2-N3	-18.27	120.17	129.30
33	BA	2812	A	N1-C2-N3	-18.26	120.17	129.30
21	AX	9	A	N1-C2-N3	-18.25	120.17	129.30
1	AA	945	A	N1-C2-N3	-18.25	120.17	129.30
33	BA	2106	A	N1-C2-N3	-18.25	120.17	129.30
33	BA	2330	A	N1-C2-N3	-18.25	120.17	129.30
33	BA	678	A	N1-C2-N3	-18.25	120.18	129.30
1	AA	1238	A	N1-C2-N3	-18.25	120.18	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	559	A	N1-C2-N3	-18.25	120.18	129.30
33	BA	866	A	N1-C2-N3	-18.25	120.18	129.30
1	AA	911	A	N1-C2-N3	-18.24	120.18	129.30
33	BA	265	A	N1-C2-N3	-18.24	120.18	129.30
1	AA	1369	A	N1-C2-N3	-18.24	120.18	129.30
33	BA	2163	A	N1-C2-N3	-18.24	120.18	129.30
33	BA	258	A	N1-C2-N3	-18.23	120.19	129.30
33	BA	56	A	N1-C2-N3	-18.22	120.19	129.30
21	AX	24	A	N1-C2-N3	-18.22	120.19	129.30
1	AA	838	A	N1-C2-N3	-18.22	120.19	129.30
33	BA	1745	A	N1-C2-N3	-18.22	120.19	129.30
33	BA	1858	A	N1-C2-N3	-18.21	120.19	129.30
1	AA	1160	A	N1-C2-N3	-18.21	120.20	129.30
33	BA	1316	A	N1-C2-N3	-18.21	120.20	129.30
1	AA	715	A	N1-C2-N3	-18.20	120.20	129.30
33	BA	1067	A	C2-N3-C4	18.20	119.70	110.60
33	BA	2862	A	N1-C2-N3	-18.20	120.20	129.30
1	AA	1256	A	N1-C2-N3	-18.20	120.20	129.30
33	BA	1067	A	N1-C2-N3	-18.20	120.20	129.30
34	BB	46	A	N1-C2-N3	-18.20	120.20	129.30
1	AA	844	A	N1-C2-N3	-18.19	120.20	129.30
33	BA	2329	A	N1-C2-N3	-18.19	120.20	129.30
33	BA	1710	A	N1-C2-N3	-18.19	120.20	129.30
33	BA	168	A	N1-C2-N3	-18.19	120.21	129.30
33	BA	1490	A	N1-C2-N3	-18.19	120.21	129.30
33	BA	2117	A	N1-C2-N3	-18.19	120.21	129.30
1	AA	1315	A	N1-C2-N3	-18.18	120.21	129.30
1	AA	364	A	N1-C2-N3	-18.18	120.21	129.30
33	BA	656	A	N1-C2-N3	-18.18	120.21	129.30
33	BA	2027	A	N1-C2-N3	-18.18	120.21	129.30
1	AA	790	A	N1-C2-N3	-18.17	120.21	129.30
33	BA	1883	A	N1-C2-N3	-18.17	120.22	129.30
33	BA	2358	A	N1-C2-N3	-18.16	120.22	129.30
1	AA	1112	A	N1-C2-N3	-18.16	120.22	129.30
33	BA	634	A	N1-C2-N3	-18.16	120.22	129.30
33	BA	2220	A	N1-C2-N3	-18.16	120.22	129.30
33	BA	974	A	N1-C2-N3	-18.15	120.22	129.30
33	BA	95	A	N1-C2-N3	-18.14	120.23	129.30
33	BA	2691	A	N1-C2-N3	-18.14	120.23	129.30
33	BA	1442	A	N1-C2-N3	-18.14	120.23	129.30
33	BA	2402	A	N1-C2-N3	-18.14	120.23	129.30
1	AA	649	A	N1-C2-N3	-18.14	120.23	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	690	A	N1-C2-N3	-18.13	120.23	129.30
1	AA	948	A	N1-C2-N3	-18.13	120.23	129.30
33	BA	52	A	N1-C2-N3	-18.12	120.24	129.30
33	BA	1103	A	N1-C2-N3	-18.11	120.24	129.30
33	BA	715	A	N1-C2-N3	-18.11	120.25	129.30
33	BA	1778	A	N1-C2-N3	-18.11	120.25	129.30
33	BA	910	A	N1-C2-N3	-18.10	120.25	129.30
33	BA	1816	A	N1-C2-N3	-18.10	120.25	129.30
1	AA	758	A	N1-C2-N3	-18.09	120.25	129.30
33	BA	501	A	C2-N3-C4	18.09	119.64	110.60
33	BA	108	A	N1-C2-N3	-18.09	120.26	129.30
33	BA	178	A	N1-C2-N3	-18.09	120.26	129.30
1	AA	959	A	N1-C2-N3	-18.08	120.26	129.30
1	AA	1278	A	N1-C2-N3	-18.08	120.26	129.30
33	BA	1839	A	N1-C2-N3	-18.08	120.26	129.30
33	BA	736	A	N1-C2-N3	-18.07	120.26	129.30
33	BA	2205	A	N1-C2-N3	-18.06	120.27	129.30
1	AA	308	A	N1-C2-N3	-18.06	120.27	129.30
33	BA	1638	A	N1-C2-N3	-18.06	120.27	129.30
33	BA	2407	A	N1-C2-N3	-18.04	120.28	129.30
1	AA	405	A	N1-C2-N3	-18.04	120.28	129.30
1	AA	507	A	N1-C2-N3	-18.03	120.28	129.30
33	BA	2123	A	N1-C2-N3	-18.03	120.28	129.30
33	BA	2436	A	N1-C2-N3	-18.02	120.29	129.30
33	BA	1006	A	N1-C2-N3	-18.02	120.29	129.30
33	BA	38	A	N1-C2-N3	-18.00	120.30	129.30
1	AA	1166	A	N1-C2-N3	-18.00	120.30	129.30
33	BA	185	A	N1-C2-N3	-18.00	120.30	129.30
33	BA	2735	A	N1-C2-N3	-18.00	120.30	129.30
33	BA	1398	A	N1-C2-N3	-17.99	120.31	129.30
33	BA	1190	A	N1-C2-N3	-17.99	120.31	129.30
1	AA	391	A	N1-C2-N3	-17.98	120.31	129.30
33	BA	1618	A	N1-C2-N3	-17.98	120.31	129.30
33	BA	1714	A	N1-C2-N3	-17.97	120.31	129.30
33	BA	679	A	N1-C2-N3	-17.96	120.32	129.30
33	BA	667	A	N1-C2-N3	-17.95	120.33	129.30
33	BA	935	A	N1-C2-N3	-17.92	120.34	129.30
33	BA	2885	A	N1-C2-N3	-17.91	120.34	129.30
33	BA	551	A	N1-C2-N3	-17.91	120.35	129.30
1	AA	1026	A	N1-C2-N3	-17.90	120.35	129.30
1	AA	933	A	N1-C2-N3	-17.87	120.36	129.30
33	BA	2844	A	N1-C2-N3	-17.85	120.38	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2627	A	N1-C2-N3	-17.84	120.38	129.30
33	BA	527	A	N1-C2-N3	-17.81	120.40	129.30
1	AA	99	A	N1-C2-N3	-17.68	120.46	129.30
33	BA	513	A	N1-C2-N3	-17.64	120.48	129.30
33	BA	254	A	N1-C2-N3	-17.11	120.75	129.30
34	BB	99	A	N1-C2-N3	-17.06	120.77	129.30
33	BA	589	G	C4'-C3'-O3'	13.94	140.88	113.00
33	BA	83	G	C4'-C3'-O3'	-12.69	82.76	109.40
33	BA	501	A	N7-C8-N9	-12.08	107.76	113.80
33	BA	2805	A	N7-C8-N9	-12.06	107.77	113.80
33	BA	526	A	N7-C8-N9	-11.94	107.83	113.80
33	BA	1134	A	N3-C4-C5	-11.93	118.45	126.80
33	BA	2089	A	N7-C8-N9	-11.92	107.84	113.80
1	AA	10	A	N7-C8-N9	-11.90	107.85	113.80
33	BA	2026	A	N7-C8-N9	-11.90	107.85	113.80
1	AA	266	A	N7-C8-N9	-11.89	107.86	113.80
33	BA	1784	A	N7-C8-N9	-11.89	107.86	113.80
33	BA	2819	A	N7-C8-N9	-11.87	107.86	113.80
33	BA	2893	A	N7-C8-N9	-11.87	107.87	113.80
33	BA	2417	A	N7-C8-N9	-11.86	107.87	113.80
33	BA	2807	A	N7-C8-N9	-11.86	107.87	113.80
33	BA	722	A	N7-C8-N9	-11.85	107.87	113.80
33	BA	1202	A	N7-C8-N9	-11.84	107.88	113.80
33	BA	847	A	N7-C8-N9	-11.84	107.88	113.80
33	BA	1555	A	N7-C8-N9	-11.83	107.88	113.80
33	BA	702	A	N7-C8-N9	-11.83	107.89	113.80
33	BA	2750	A	N7-C8-N9	-11.83	107.89	113.80
1	AA	508	A	N7-C8-N9	-11.83	107.89	113.80
33	BA	1189	A	N7-C8-N9	-11.82	107.89	113.80
1	AA	703	A	N7-C8-N9	-11.82	107.89	113.80
33	BA	1473	A	N7-C8-N9	-11.82	107.89	113.80
1	AA	556	A	N7-C8-N9	-11.81	107.89	113.80
1	AA	1065	A	N7-C8-N9	-11.81	107.89	113.80
33	BA	821	A	N7-C8-N9	-11.81	107.89	113.80
33	BA	1895	A	N7-C8-N9	-11.81	107.89	113.80
33	BA	2447	A	N7-C8-N9	-11.81	107.89	113.80
1	AA	254	A	N7-C8-N9	-11.80	107.90	113.80
33	BA	374	A	N7-C8-N9	-11.80	107.90	113.80
33	BA	1084	A	N7-C8-N9	-11.80	107.90	113.80
33	BA	1815	A	N7-C8-N9	-11.79	107.91	113.80
1	AA	862	A	N7-C8-N9	-11.78	107.91	113.80
33	BA	1302	A	N7-C8-N9	-11.78	107.91	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1417	A	N7-C8-N9	-11.77	107.91	113.80
1	AA	790	A	N7-C8-N9	-11.77	107.92	113.80
1	AA	985	A	N7-C8-N9	-11.76	107.92	113.80
33	BA	1061	A	N7-C8-N9	-11.76	107.92	113.80
33	BA	2777	A	N7-C8-N9	-11.76	107.92	113.80
1	AA	1434	A	N7-C8-N9	-11.76	107.92	113.80
33	BA	207	A	N7-C8-N9	-11.76	107.92	113.80
33	BA	1003	A	N7-C8-N9	-11.76	107.92	113.80
1	AA	899	A	N7-C8-N9	-11.75	107.92	113.80
33	BA	774	A	N7-C8-N9	-11.75	107.92	113.80
33	BA	835	A	N7-C8-N9	-11.75	107.92	113.80
33	BA	2187	A	N7-C8-N9	-11.75	107.92	113.80
33	BA	647	A	N7-C8-N9	-11.75	107.92	113.80
33	BA	1314	A	N7-C8-N9	-11.75	107.92	113.80
1	AA	419	A	N7-C8-N9	-11.75	107.93	113.80
33	BA	2670	A	N7-C8-N9	-11.75	107.93	113.80
1	AA	768	A	N7-C8-N9	-11.74	107.93	113.80
1	AA	923	A	N7-C8-N9	-11.74	107.93	113.80
33	BA	2155	A	N7-C8-N9	-11.74	107.93	113.80
33	BA	538	A	N7-C8-N9	-11.74	107.93	113.80
33	BA	1161	A	N7-C8-N9	-11.74	107.93	113.80
33	BA	1325	A	N7-C8-N9	-11.74	107.93	113.80
1	AA	1355	A	N7-C8-N9	-11.74	107.93	113.80
33	BA	504	A	N7-C8-N9	-11.74	107.93	113.80
1	AA	94	A	N7-C8-N9	-11.73	107.93	113.80
1	AA	206	A	N7-C8-N9	-11.73	107.93	113.80
33	BA	1034	A	N7-C8-N9	-11.73	107.93	113.80
33	BA	2170	A	N7-C8-N9	-11.73	107.93	113.80
33	BA	1308	A	N7-C8-N9	-11.73	107.94	113.80
33	BA	1982	A	N7-C8-N9	-11.73	107.94	113.80
33	BA	2683	A	N7-C8-N9	-11.72	107.94	113.80
1	AA	879	A	N7-C8-N9	-11.72	107.94	113.80
33	BA	575	A	N7-C8-N9	-11.72	107.94	113.80
33	BA	2362	A	N7-C8-N9	-11.72	107.94	113.80
33	BA	2770	A	N7-C8-N9	-11.72	107.94	113.80
1	AA	1077	A	N7-C8-N9	-11.72	107.94	113.80
33	BA	1461	A	N7-C8-N9	-11.72	107.94	113.80
33	BA	2152	A	N7-C8-N9	-11.72	107.94	113.80
1	AA	988	A	N7-C8-N9	-11.71	107.94	113.80
33	BA	64	A	N7-C8-N9	-11.71	107.94	113.80
33	BA	1339	A	N7-C8-N9	-11.71	107.94	113.80
1	AA	925	A	N7-C8-N9	-11.71	107.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	324	A	N7-C8-N9	-11.71	107.94	113.80
33	BA	584	A	N7-C8-N9	-11.71	107.95	113.80
33	BA	1305	A	N7-C8-N9	-11.71	107.95	113.80
33	BA	2601	A	N7-C8-N9	-11.71	107.95	113.80
33	BA	1654	A	N7-C8-N9	-11.71	107.95	113.80
34	BB	17	A	N7-C8-N9	-11.71	107.95	113.80
1	AA	1225	A	N7-C8-N9	-11.70	107.95	113.80
33	BA	421	A	N7-C8-N9	-11.70	107.95	113.80
33	BA	2315	A	N7-C8-N9	-11.70	107.95	113.80
1	AA	1248	A	N7-C8-N9	-11.70	107.95	113.80
33	BA	281	A	N7-C8-N9	-11.70	107.95	113.80
33	BA	322	A	N7-C8-N9	-11.70	107.95	113.80
33	BA	2088	A	N7-C8-N9	-11.70	107.95	113.80
1	AA	57	A	N7-C8-N9	-11.70	107.95	113.80
33	BA	1809	A	N7-C8-N9	-11.70	107.95	113.80
33	BA	2254	A	N7-C8-N9	-11.70	107.95	113.80
33	BA	2594	A	N7-C8-N9	-11.69	107.95	113.80
1	AA	456	A	N7-C8-N9	-11.69	107.95	113.80
1	AA	824	A	N7-C8-N9	-11.69	107.95	113.80
1	AA	1466	A	N7-C8-N9	-11.69	107.95	113.80
1	AA	422	A	N7-C8-N9	-11.69	107.95	113.80
33	BA	999	A	N7-C8-N9	-11.69	107.95	113.80
33	BA	2923	A	N7-C8-N9	-11.69	107.95	113.80
33	BA	154	A	N7-C8-N9	-11.69	107.96	113.80
33	BA	1047	A	N7-C8-N9	-11.69	107.96	113.80
33	BA	2134	A	N7-C8-N9	-11.69	107.96	113.80
1	AA	189	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	1488	A	N7-C8-N9	-11.68	107.96	113.80
33	BA	1094	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	202	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	1503	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	886	A	N7-C8-N9	-11.68	107.96	113.80
33	BA	1700	A	N7-C8-N9	-11.68	107.96	113.80
33	BA	1326	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	786	A	N7-C8-N9	-11.67	107.96	113.80
33	BA	991	A	N7-C8-N9	-11.67	107.96	113.80
33	BA	2390	A	N7-C8-N9	-11.67	107.97	113.80
33	BA	2618	A	N7-C8-N9	-11.67	107.97	113.80
33	BA	1014	A	N7-C8-N9	-11.67	107.97	113.80
33	BA	572	A	N7-C8-N9	-11.66	107.97	113.80
33	BA	2907	A	N7-C8-N9	-11.66	107.97	113.80
33	BA	582	A	N7-C8-N9	-11.66	107.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	876	A	N7-C8-N9	-11.66	107.97	113.80
33	BA	2673	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	228	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	452	A	N7-C8-N9	-11.66	107.97	113.80
33	BA	71	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	1541	A	N7-C8-N9	-11.66	107.97	113.80
33	BA	618	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	364	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	1257	A	N7-C8-N9	-11.66	107.97	113.80
33	BA	1224	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	159	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	415	A	N7-C8-N9	-11.65	107.97	113.80
33	BA	28	A	N7-C8-N9	-11.65	107.97	113.80
33	BA	1424	A	N7-C8-N9	-11.65	107.97	113.80
33	BA	150	A	N7-C8-N9	-11.65	107.97	113.80
33	BA	229	A	N7-C8-N9	-11.65	107.97	113.80
33	BA	525	A	N7-C8-N9	-11.65	107.97	113.80
33	BA	2876	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	203	A	N7-C8-N9	-11.65	107.97	113.80
33	BA	1585	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	204	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	1222	A	N7-C8-N9	-11.65	107.97	113.80
33	BA	690	A	N7-C8-N9	-11.65	107.97	113.80
33	BA	1254	A	N7-C8-N9	-11.65	107.97	113.80
33	BA	2062	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	53	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	1407	A	N7-C8-N9	-11.65	107.98	113.80
33	BA	389	A	N7-C8-N9	-11.65	107.98	113.80
33	BA	1483	A	N7-C8-N9	-11.65	107.98	113.80
1	AA	460	A	N7-C8-N9	-11.64	107.98	113.80
1	AA	1456	A	N7-C8-N9	-11.64	107.98	113.80
33	BA	183	A	N7-C8-N9	-11.64	107.98	113.80
33	BA	2049	A	N7-C8-N9	-11.64	107.98	113.80
33	BA	126	A	N7-C8-N9	-11.64	107.98	113.80
33	BA	646	A	N7-C8-N9	-11.64	107.98	113.80
33	BA	1735	A	N7-C8-N9	-11.64	107.98	113.80
33	BA	2059	A	N7-C8-N9	-11.64	107.98	113.80
33	BA	2398	A	N7-C8-N9	-11.64	107.98	113.80
1	AA	737	A	N7-C8-N9	-11.64	107.98	113.80
33	BA	307	A	N7-C8-N9	-11.64	107.98	113.80
33	BA	1966	A	N7-C8-N9	-11.64	107.98	113.80
1	AA	1386	A	N7-C8-N9	-11.64	107.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1277	A	N7-C8-N9	-11.64	107.98	113.80
1	AA	62	A	N7-C8-N9	-11.63	107.98	113.80
33	BA	2902	A	N7-C8-N9	-11.63	107.98	113.80
1	AA	522	A	N7-C8-N9	-11.63	107.98	113.80
1	AA	690	A	N7-C8-N9	-11.63	107.99	113.80
33	BA	490	A	N7-C8-N9	-11.63	107.99	113.80
33	BA	1998	A	N7-C8-N9	-11.63	107.99	113.80
33	BA	1008	A	N7-C8-N9	-11.63	107.99	113.80
1	AA	1006	A	N7-C8-N9	-11.63	107.99	113.80
1	AA	1185	A	N7-C8-N9	-11.63	107.99	113.80
1	AA	240	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	236	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	412	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	1347	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	2071	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	31	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	730	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	959	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	2455	A	N7-C8-N9	-11.62	107.99	113.80
34	BB	114	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	650	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	1210	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	1512	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	244	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	1464	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	2276	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	190	A	N7-C8-N9	-11.61	107.99	113.80
1	AA	672	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	811	A	N7-C8-N9	-11.61	107.99	113.80
1	AA	1213	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	1298	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	110	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	140	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	166	A	N7-C8-N9	-11.62	107.99	113.80
33	BA	882	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	18	A	N7-C8-N9	-11.61	107.99	113.80
1	AA	232	A	N7-C8-N9	-11.61	107.99	113.80
33	BA	325	A	N7-C8-N9	-11.61	107.99	113.80
1	AA	658	A	N7-C8-N9	-11.61	108.00	113.80
33	BA	314	A	N7-C8-N9	-11.61	107.99	113.80
33	BA	1157	A	N7-C8-N9	-11.61	108.00	113.80
33	BA	1553	A	N7-C8-N9	-11.61	108.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2854	A	N7-C8-N9	-11.61	107.99	113.80
1	AA	651	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	1513	A	N7-C8-N9	-11.61	108.00	113.80
33	BA	194	A	N7-C8-N9	-11.61	108.00	113.80
33	BA	1287	A	N7-C8-N9	-11.61	108.00	113.80
33	BA	2782	A	N7-C8-N9	-11.61	108.00	113.80
33	BA	1967	A	N7-C8-N9	-11.61	108.00	113.80
33	BA	2860	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	532	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	1328	A	N7-C8-N9	-11.61	108.00	113.80
33	BA	2835	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	440	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	506	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	677	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	1188	A	N7-C8-N9	-11.60	108.00	113.80
33	BA	888	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	1422	A	N7-C8-N9	-11.60	108.00	113.80
33	BA	376	A	N7-C8-N9	-11.60	108.00	113.80
33	BA	1144	A	N7-C8-N9	-11.60	108.00	113.80
33	BA	1233	A	N7-C8-N9	-11.60	108.00	113.80
33	BA	2846	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	386	A	N7-C8-N9	-11.60	108.00	113.80
33	BA	219	A	N7-C8-N9	-11.60	108.00	113.80
33	BA	2542	A	N7-C8-N9	-11.60	108.00	113.80
33	BA	224	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	118	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	357	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	777	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	569	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	611	A	N7-C8-N9	-11.60	108.00	113.80
33	BA	260	A	N7-C8-N9	-11.60	108.00	113.80
33	BA	2317	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	382	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	704	A	N7-C8-N9	-11.59	108.00	113.80
33	BA	1504	A	N7-C8-N9	-11.59	108.00	113.80
33	BA	2052	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	371	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	910	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	1348	A	N7-C8-N9	-11.59	108.00	113.80
33	BA	957	A	N7-C8-N9	-11.59	108.00	113.80
33	BA	1648	A	N7-C8-N9	-11.59	108.00	113.80
33	BA	2216	A	N7-C8-N9	-11.59	108.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1925	A	N7-C8-N9	-11.59	108.00	113.80
33	BA	2500	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	281	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	671	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	803	A	N7-C8-N9	-11.59	108.00	113.80
33	BA	1175	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	544	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	568	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	1320	A	N7-C8-N9	-11.59	108.01	113.80
33	BA	530	A	N7-C8-N9	-11.59	108.01	113.80
33	BA	1914	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	178	A	N7-C8-N9	-11.59	108.01	113.80
33	BA	2302	A	N7-C8-N9	-11.59	108.01	113.80
33	BA	2364	A	N7-C8-N9	-11.59	108.01	113.80
33	BA	2365	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	361	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1056	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1176	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	216	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	1115	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	1813	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	2356	A	N7-C8-N9	-11.58	108.01	113.80
34	BB	39	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1092	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	619	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	1142	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	2908	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1528	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	274	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	500	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1090	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1178	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	1266	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	1406	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	2262	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	723	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	1901	A	N7-C8-N9	-11.58	108.01	113.80
33	BA	2464	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	542	A	N7-C8-N9	-11.57	108.01	113.80
33	BA	202	A	N7-C8-N9	-11.57	108.01	113.80
33	BA	354	A	N7-C8-N9	-11.57	108.01	113.80
33	BA	1516	A	N7-C8-N9	-11.57	108.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2042	A	N7-C8-N9	-11.57	108.01	113.80
1	AA	618	A	N7-C8-N9	-11.57	108.01	113.80
1	AA	1133	A	N7-C8-N9	-11.57	108.01	113.80
33	BA	1679	A	N7-C8-N9	-11.57	108.01	113.80
33	BA	1961	A	N7-C8-N9	-11.57	108.01	113.80
33	BA	2338	A	N7-C8-N9	-11.57	108.01	113.80
33	BA	2507	A	N7-C8-N9	-11.57	108.01	113.80
33	BA	2694	A	N7-C8-N9	-11.57	108.01	113.80
33	BA	717	A	N7-C8-N9	-11.57	108.02	113.80
1	AA	816	A	N7-C8-N9	-11.57	108.02	113.80
1	AA	1479	A	N7-C8-N9	-11.57	108.02	113.80
33	BA	947	A	N7-C8-N9	-11.57	108.02	113.80
33	BA	1743	A	N7-C8-N9	-11.57	108.02	113.80
33	BA	125	A	N7-C8-N9	-11.57	108.02	113.80
33	BA	333	A	N7-C8-N9	-11.57	108.02	113.80
33	BA	1524	A	N7-C8-N9	-11.57	108.02	113.80
33	BA	1948	A	N7-C8-N9	-11.57	108.02	113.80
33	BA	2722	A	N7-C8-N9	-11.57	108.02	113.80
34	BB	25	A	N7-C8-N9	-11.57	108.02	113.80
1	AA	664	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	278	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	2700	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	364	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	388	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	1269	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	2256	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	501	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	1417	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	500	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	763	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	868	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	1913	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	2708	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	776	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	952	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	1126	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	234	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	258	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	282	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	2119	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	738	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	947	A	N7-C8-N9	-11.56	108.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1271	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	1419	A	N7-C8-N9	-11.56	108.02	113.80
33	BA	2298	A	N7-C8-N9	-11.56	108.02	113.80
34	BB	27	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	1205	A	N7-C8-N9	-11.55	108.02	113.80
1	AA	1383	A	N7-C8-N9	-11.56	108.02	113.80
21	AX	41	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	919	A	N7-C8-N9	-11.55	108.02	113.80
1	AA	1050	A	N7-C8-N9	-11.55	108.02	113.80
1	AA	1252	A	N7-C8-N9	-11.55	108.02	113.80
33	BA	2482	A	N7-C8-N9	-11.55	108.02	113.80
33	BA	2912	A	N7-C8-N9	-11.55	108.02	113.80
33	BA	637	A	N7-C8-N9	-11.55	108.02	113.80
33	BA	67	A	N7-C8-N9	-11.55	108.03	113.80
33	BA	133	A	N7-C8-N9	-11.55	108.03	113.80
33	BA	337	A	N7-C8-N9	-11.55	108.02	113.80
33	BA	2241	A	N7-C8-N9	-11.55	108.02	113.80
33	BA	1686	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	148	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	496	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	679	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	837	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	1451	A	N7-C8-N9	-11.55	108.03	113.80
33	BA	507	A	N7-C8-N9	-11.55	108.03	113.80
33	BA	1942	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	771	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	828	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	1443	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	978	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	1210	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	1375	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	2047	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	2330	A	N7-C8-N9	-11.55	108.03	113.80
33	BA	2668	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	463	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	928	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	1020	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	459	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	2340	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	296	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	321	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	367	A	N7-C8-N9	-11.54	108.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	616	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1102	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1256	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	770	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	1131	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	2851	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	389	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	345	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	758	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	965	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	2375	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	2686	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	2837	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	423	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	757	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1349	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1510	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	1906	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1197	A	N7-C8-N9	-11.53	108.03	113.80
33	BA	94	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	519	A	N7-C8-N9	-11.53	108.03	113.80
33	BA	677	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	1123	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	1230	A	N7-C8-N9	-11.54	108.03	113.80
33	BA	1291	A	N7-C8-N9	-11.53	108.03	113.80
33	BA	1432	A	N7-C8-N9	-11.53	108.03	113.80
33	BA	2658	A	N7-C8-N9	-11.53	108.03	113.80
21	AX	58	A	N7-C8-N9	-11.53	108.03	113.80
33	BA	547	A	N7-C8-N9	-11.53	108.03	113.80
33	BA	1947	A	N7-C8-N9	-11.53	108.03	113.80
33	BA	2307	A	N7-C8-N9	-11.53	108.03	113.80
34	BB	51	A	N7-C8-N9	-11.53	108.03	113.80
33	BA	786	A	N7-C8-N9	-11.53	108.03	113.80
33	BA	1797	A	N7-C8-N9	-11.53	108.03	113.80
33	BA	2083	A	N7-C8-N9	-11.53	108.03	113.80
1	AA	762	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	831	A	N7-C8-N9	-11.53	108.04	113.80
33	BA	553	A	N7-C8-N9	-11.53	108.04	113.80
33	BA	736	A	N7-C8-N9	-11.53	108.04	113.80
33	BA	917	A	N7-C8-N9	-11.53	108.04	113.80
33	BA	1078	A	N7-C8-N9	-11.53	108.04	113.80
33	BA	1116	A	N7-C8-N9	-11.53	108.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1201	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	211	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	251	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	401	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	791	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	870	A	N7-C8-N9	-11.53	108.04	113.80
21	AX	21	A	N7-C8-N9	-11.53	108.04	113.80
34	BB	44	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	491	A	N7-C8-N9	-11.53	108.04	113.80
33	BA	144	A	N7-C8-N9	-11.53	108.04	113.80
33	BA	1592	A	N7-C8-N9	-11.53	108.04	113.80
33	BA	2787	A	N7-C8-N9	-11.53	108.04	113.80
33	BA	2810	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	139	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	329	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	2462	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	529	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	541	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1028	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	302	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	429	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	518	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	781	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	2297	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1254	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	1392	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	1713	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	2132	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1022	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1509	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	578	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	2295	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	2767	A	N7-C8-N9	-11.52	108.04	113.80
34	BB	18	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	278	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	404	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1529	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	369	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	808	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	1631	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	236	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	1174	A	N7-C8-N9	-11.52	108.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1746	A	N7-C8-N9	-11.52	108.04	113.80
33	BA	1802	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	142	A	N7-C8-N9	-11.51	108.04	113.80
1	AA	208	A	N7-C8-N9	-11.51	108.04	113.80
1	AA	1121	A	N7-C8-N9	-11.51	108.04	113.80
1	AA	1333	A	N7-C8-N9	-11.51	108.04	113.80
1	AA	1470	A	N7-C8-N9	-11.51	108.04	113.80
34	BB	97	A	N7-C8-N9	-11.51	108.04	113.80
33	BA	549	A	N7-C8-N9	-11.51	108.04	113.80
33	BA	782	A	N7-C8-N9	-11.51	108.04	113.80
33	BA	1141	A	N7-C8-N9	-11.51	108.04	113.80
33	BA	2087	A	N7-C8-N9	-11.51	108.04	113.80
33	BA	2163	A	N7-C8-N9	-11.51	108.04	113.80
1	AA	34	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	107	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	605	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	1207	A	N7-C8-N9	-11.51	108.04	113.80
33	BA	543	A	N7-C8-N9	-11.51	108.05	113.80
33	BA	1113	A	N7-C8-N9	-11.51	108.05	113.80
21	AX	14	A	N7-C8-N9	-11.51	108.05	113.80
33	BA	418	A	N7-C8-N9	-11.51	108.05	113.80
33	BA	1844	A	N7-C8-N9	-11.51	108.05	113.80
33	BA	2812	A	N7-C8-N9	-11.51	108.05	113.80
33	BA	2889	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	592	A	N7-C8-N9	-11.51	108.05	113.80
33	BA	173	A	N7-C8-N9	-11.51	108.05	113.80
33	BA	1699	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	975	A	N7-C8-N9	-11.51	108.05	113.80
33	BA	1179	A	N7-C8-N9	-11.51	108.05	113.80
33	BA	2007	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	150	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	318	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	2477	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	617	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	1357	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	2479	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	1532	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	2719	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	346	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	669	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	1115	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	2034	A	N7-C8-N9	-11.50	108.05	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1327	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	1059	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	67	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	117	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	306	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	161	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	225	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	448	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	1284	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	1312	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	1517	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	1593	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	2754	A	N7-C8-N9	-11.50	108.05	113.80
33	BA	2830	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	1245	A	N7-C8-N9	-11.49	108.05	113.80
33	BA	124	A	N7-C8-N9	-11.49	108.05	113.80
1	AA	1048	A	N7-C8-N9	-11.49	108.05	113.80
1	AA	1523	A	N7-C8-N9	-11.49	108.05	113.80
33	BA	353	A	N7-C8-N9	-11.49	108.05	113.80
33	BA	1072	A	N7-C8-N9	-11.49	108.05	113.80
33	BA	1323	A	N7-C8-N9	-11.49	108.05	113.80
33	BA	1243	A	N7-C8-N9	-11.49	108.05	113.80
33	BA	2220	A	N7-C8-N9	-11.49	108.05	113.80
34	BB	55	A	N7-C8-N9	-11.49	108.05	113.80
33	BA	84	A	N7-C8-N9	-11.49	108.06	113.80
33	BA	193	A	N7-C8-N9	-11.49	108.06	113.80
33	BA	1405	A	N7-C8-N9	-11.49	108.06	113.80
33	BA	1540	A	N7-C8-N9	-11.49	108.05	113.80
33	BA	2769	A	N7-C8-N9	-11.49	108.05	113.80
33	BA	2793	A	N7-C8-N9	-11.49	108.05	113.80
33	BA	1025	A	N7-C8-N9	-11.49	108.06	113.80
33	BA	1663	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	287	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	801	A	N7-C8-N9	-11.49	108.06	113.80
33	BA	355	A	N7-C8-N9	-11.49	108.06	113.80
33	BA	436	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	329	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	333	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	1160	A	N7-C8-N9	-11.49	108.06	113.80
33	BA	171	A	N7-C8-N9	-11.49	108.06	113.80
33	BA	829	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	1486	A	N7-C8-N9	-11.49	108.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	5	A	N7-C8-N9	-11.49	108.06	113.80
33	BA	652	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	799	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	139	A	N7-C8-N9	-11.48	108.06	113.80
34	BB	76	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	956	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1259	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	475	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	1286	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	1534	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	1615	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	1066	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	2571	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1455	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1490	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	6	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	49	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	2191	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	2505	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	485	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	2000	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	924	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	974	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	1437	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	561	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	1026	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	1789	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	2629	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	653	A	N7-C8-N9	-11.48	108.06	113.80
33	BA	769	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	638	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	2030	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	796	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	1284	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	893	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	1194	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	1675	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	1677	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	1691	A	N3-C4-C5	-11.47	118.77	126.80
33	BA	1812	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	2148	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	2165	A	N7-C8-N9	-11.47	108.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	43	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	1147	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	1289	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	1502	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	1313	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	2018	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	1423	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	129	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	504	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	512	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	1054	A	N7-C8-N9	-11.47	108.07	113.80
33	BA	305	A	N7-C8-N9	-11.47	108.06	113.80
33	BA	470	A	N7-C8-N9	-11.47	108.07	113.80
33	BA	2421	A	N7-C8-N9	-11.47	108.06	113.80
1	AA	1120	A	N7-C8-N9	-11.47	108.07	113.80
33	BA	210	A	N7-C8-N9	-11.47	108.07	113.80
33	BA	273	A	N7-C8-N9	-11.47	108.07	113.80
33	BA	1533	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	61	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	2919	A	N7-C8-N9	-11.47	108.07	113.80
1	AA	160	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	1369	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	476	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	752	A	N7-C8-N9	-11.47	108.07	113.80
33	BA	1412	A	N7-C8-N9	-11.47	108.07	113.80
33	BA	1845	A	N7-C8-N9	-11.47	108.07	113.80
33	BA	922	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	1608	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	81	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	1103	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	1493	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	120	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	582	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	696	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	811	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	1055	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	1335	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	225	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	1296	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	1636	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	1685	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	1722	A	N7-C8-N9	-11.46	108.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	838	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	13	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	200	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	974	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	1929	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	173	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	685	A	N7-C8-N9	-11.45	108.07	113.80
33	BA	428	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	1520	A	N7-C8-N9	-11.46	108.07	113.80
33	BA	740	A	N7-C8-N9	-11.45	108.07	113.80
33	BA	2383	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	917	A	N7-C8-N9	-11.45	108.07	113.80
1	AA	1206	A	N7-C8-N9	-11.45	108.07	113.80
33	BA	12	A	N7-C8-N9	-11.45	108.07	113.80
33	BA	600	A	N7-C8-N9	-11.45	108.07	113.80
33	BA	724	A	N7-C8-N9	-11.45	108.07	113.80
33	BA	2043	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	2369	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	2904	A	N7-C8-N9	-11.45	108.07	113.80
34	BB	64	A	N7-C8-N9	-11.45	108.07	113.80
1	AA	210	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	433	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	1017	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	1247	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	179	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	1197	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	2762	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	1588	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	475	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	604	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	1112	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	1270	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	14	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	705	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	1575	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	1653	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	2100	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	2200	A	N7-C8-N9	-11.45	108.08	113.80
33	BA	2734	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	170	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1111	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1260	A	N7-C8-N9	-11.44	108.08	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	762	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	1445	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	1734	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	342	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	721	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	1918	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	2329	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	2461	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	12	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	28	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	323	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1180	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	226	A	N3-C4-C5	-11.44	118.79	126.80
33	BA	326	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	1029	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	1838	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	2343	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	2606	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1359	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1140	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	449	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	867	A	N7-C8-N9	-11.44	108.08	113.80
33	BA	1672	A	N7-C8-N9	-11.44	108.08	113.80
34	BB	102	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1405	A	N7-C8-N9	-11.43	108.08	113.80
33	BA	456	A	N7-C8-N9	-11.43	108.08	113.80
33	BA	987	A	N7-C8-N9	-11.43	108.08	113.80
33	BA	1021	A	N7-C8-N9	-11.43	108.08	113.80
33	BA	2875	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	290	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	775	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	823	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	151	A	N7-C8-N9	-11.43	108.09	113.80
1	AA	335	A	N7-C8-N9	-11.43	108.08	113.80
33	BA	65	A	N7-C8-N9	-11.43	108.08	113.80
33	BA	551	A	N7-C8-N9	-11.43	108.08	113.80
33	BA	715	A	N7-C8-N9	-11.43	108.08	113.80
33	BA	870	A	N7-C8-N9	-11.43	108.08	113.80
33	BA	1346	A	N7-C8-N9	-11.43	108.08	113.80
33	BA	1957	A	N7-C8-N9	-11.43	108.08	113.80
21	AX	44	A	N7-C8-N9	-11.43	108.09	113.80
33	BA	828	A	N7-C8-N9	-11.43	108.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2124	A	N7-C8-N9	-11.43	108.09	113.80
1	AA	979	A	N7-C8-N9	-11.43	108.09	113.80
1	AA	659	A	N7-C8-N9	-11.43	108.09	113.80
33	BA	102	A	N7-C8-N9	-11.43	108.09	113.80
33	BA	330	A	N7-C8-N9	-11.43	108.09	113.80
33	BA	373	A	N7-C8-N9	-11.43	108.09	113.80
33	BA	1190	A	N7-C8-N9	-11.43	108.09	113.80
33	BA	1092	A	N7-C8-N9	-11.43	108.09	113.80
33	BA	1788	A	N7-C8-N9	-11.43	108.09	113.80
33	BA	1818	A	N7-C8-N9	-11.43	108.09	113.80
33	BA	2526	A	N7-C8-N9	-11.43	108.09	113.80
33	BA	2643	A	N7-C8-N9	-11.43	108.09	113.80
1	AA	631	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	1425	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	2898	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	1042	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	1490	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	1617	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	1995	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	199	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	1477	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	993	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	1745	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	674	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	1358	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	1442	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	945	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	1149	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	1791	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	1583	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	2661	A	N7-C8-N9	-11.42	108.09	113.80
33	BA	1119	A	N7-C8-N9	-11.41	108.09	113.80
33	BA	2804	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	918	A	N7-C8-N9	-11.41	108.09	113.80
33	BA	1989	A	N7-C8-N9	-11.41	108.09	113.80
33	BA	2327	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	55	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	171	A	N7-C8-N9	-11.41	108.09	113.80
33	BA	222	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	352	A	N7-C8-N9	-11.41	108.09	113.80
33	BA	1130	A	N7-C8-N9	-11.41	108.09	113.80
33	BA	2845	A	N7-C8-N9	-11.41	108.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	176	A	N7-C8-N9	-11.41	108.10	113.80
33	BA	1046	A	N7-C8-N9	-11.41	108.10	113.80
33	BA	1727	A	N7-C8-N9	-11.41	108.10	113.80
33	BA	1941	A	N7-C8-N9	-11.41	108.10	113.80
33	BA	2402	A	N7-C8-N9	-11.41	108.10	113.80
1	AA	314	A	N7-C8-N9	-11.41	108.10	113.80
33	BA	1638	A	N7-C8-N9	-11.41	108.10	113.80
33	BA	2078	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	35	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	2146	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	889	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	970	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	1776	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	2387	A	N7-C8-N9	-11.40	108.10	113.80
34	BB	56	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	344	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	397	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	1235	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	2032	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	2381	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	2498	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	793	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	715	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	108	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	486	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	1253	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	1499	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	1695	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	2270	A	N7-C8-N9	-11.40	108.10	113.80
33	BA	41	A	N7-C8-N9	-11.39	108.10	113.80
33	BA	479	A	N7-C8-N9	-11.39	108.10	113.80
33	BA	1005	A	N7-C8-N9	-11.39	108.10	113.80
33	BA	2619	A	N7-C8-N9	-11.39	108.10	113.80
33	BA	2662	A	N7-C8-N9	-11.39	108.10	113.80
33	BA	964	A	N7-C8-N9	-11.39	108.10	113.80
1	AA	1004	A	N7-C8-N9	-11.39	108.11	113.80
33	BA	73	A	N7-C8-N9	-11.39	108.11	113.80
33	BA	259	A	N7-C8-N9	-11.39	108.11	113.80
33	BA	1036	A	N7-C8-N9	-11.39	108.10	113.80
33	BA	2117	A	N7-C8-N9	-11.39	108.11	113.80
1	AA	438	A	N7-C8-N9	-11.39	108.11	113.80
1	AA	1403	A	N7-C8-N9	-11.39	108.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2316	A	N7-C8-N9	-11.39	108.11	113.80
33	BA	2590	A	N7-C8-N9	-11.39	108.11	113.80
33	BA	2740	A	N7-C8-N9	-11.39	108.11	113.80
1	AA	883	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	1434	A	N7-C8-N9	-11.39	108.11	113.80
1	AA	1200	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	230	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	2027	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	1054	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	52	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	198	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	206	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	231	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	469	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	1404	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	2663	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	474	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	517	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	851	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	1100	A	N7-C8-N9	-11.38	108.11	113.80
34	BB	105	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1014	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	156	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	1627	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	1831	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1342	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1384	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	130	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	727	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	1258	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	1260	A	N7-C8-N9	-11.38	108.11	113.80
33	BA	2454	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	76	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	271	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	372	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	649	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	978	A	N7-C8-N9	-11.37	108.11	113.80
33	BA	1381	A	N7-C8-N9	-11.37	108.11	113.80
33	BA	1426	A	N7-C8-N9	-11.37	108.11	113.80
33	BA	1465	A	N7-C8-N9	-11.37	108.11	113.80
33	BA	1569	A	N7-C8-N9	-11.37	108.11	113.80
33	BA	2547	A	N7-C8-N9	-11.37	108.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	37	A	N7-C8-N9	-11.37	108.11	113.80
33	BA	866	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	72	A	N7-C8-N9	-11.37	108.12	113.80
33	BA	21	A	N7-C8-N9	-11.37	108.12	113.80
33	BA	592	A	N7-C8-N9	-11.37	108.12	113.80
33	BA	1723	A	N7-C8-N9	-11.37	108.11	113.80
33	BA	2900	A	N7-C8-N9	-11.37	108.11	113.80
33	BA	524	A	N7-C8-N9	-11.37	108.12	113.80
33	BA	683	A	N7-C8-N9	-11.37	108.12	113.80
33	BA	2080	A	N7-C8-N9	-11.37	108.12	113.80
1	AA	301	A	N7-C8-N9	-11.37	108.12	113.80
33	BA	44	A	N7-C8-N9	-11.37	108.12	113.80
1	AA	462	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	1580	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	2006	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	2227	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	2790	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	2834	A	N7-C8-N9	-11.37	108.12	113.80
1	AA	507	A	N7-C8-N9	-11.36	108.12	113.80
1	AA	581	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	258	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	753	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	2570	A	N7-C8-N9	-11.36	108.12	113.80
34	BB	113	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	2511	A	N7-C8-N9	-11.36	108.12	113.80
34	BB	50	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	2066	A	N7-C8-N9	-11.36	108.12	113.80
1	AA	140	A	N7-C8-N9	-11.36	108.12	113.80
33	BA	1760	A	N7-C8-N9	-11.35	108.12	113.80
33	BA	10	A	N7-C8-N9	-11.35	108.12	113.80
33	BA	279	A	N7-C8-N9	-11.35	108.12	113.80
33	BA	746	A	N7-C8-N9	-11.35	108.12	113.80
33	BA	1541	A	N7-C8-N9	-11.35	108.12	113.80
33	BA	1981	A	N7-C8-N9	-11.35	108.12	113.80
33	BA	2351	A	N7-C8-N9	-11.35	108.12	113.80
33	BA	548	A	N7-C8-N9	-11.35	108.12	113.80
1	AA	459	A	N7-C8-N9	-11.35	108.13	113.80
1	AA	705	A	N7-C8-N9	-11.35	108.13	113.80
33	BA	1710	A	N7-C8-N9	-11.35	108.13	113.80
33	BA	2887	A	N7-C8-N9	-11.34	108.13	113.80
33	BA	2924	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	1435	A	N7-C8-N9	-11.34	108.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	220	A	N7-C8-N9	-11.34	108.13	113.80
33	BA	2389	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	270	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	381	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	684	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	902	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	1308	A	N3-C4-C5	-11.34	118.86	126.80
33	BA	659	A	N7-C8-N9	-11.34	108.13	113.80
21	AX	70	A	N7-C8-N9	-11.34	108.13	113.80
33	BA	162	A	N7-C8-N9	-11.34	108.13	113.80
33	BA	407	A	N7-C8-N9	-11.34	108.13	113.80
33	BA	1316	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	913	A	N7-C8-N9	-11.34	108.13	113.80
33	BA	1027	A	N7-C8-N9	-11.34	108.13	113.80
21	AX	76	A	N7-C8-N9	-11.33	108.13	113.80
33	BA	1442	A	N7-C8-N9	-11.33	108.13	113.80
1	AA	337	A	N7-C8-N9	-11.33	108.14	113.80
33	BA	265	A	N7-C8-N9	-11.33	108.14	113.80
33	BA	896	A	N7-C8-N9	-11.33	108.13	113.80
33	BA	2406	A	N7-C8-N9	-11.33	108.14	113.80
33	BA	537	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	825	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	1517	A	N7-C8-N9	-11.33	108.14	113.80
33	BA	692	A	N7-C8-N9	-11.33	108.14	113.80
33	BA	1876	A	N7-C8-N9	-11.33	108.14	113.80
1	AA	968	A	N7-C8-N9	-11.32	108.14	113.80
33	BA	667	A	N7-C8-N9	-11.32	108.14	113.80
33	BA	910	A	N7-C8-N9	-11.32	108.14	113.80
33	BA	1579	A	N7-C8-N9	-11.32	108.14	113.80
33	BA	2405	A	N7-C8-N9	-11.32	108.14	113.80
34	BB	46	A	N7-C8-N9	-11.32	108.14	113.80
33	BA	1542	A	N7-C8-N9	-11.32	108.14	113.80
34	BB	71	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	1024	A	N7-C8-N9	-11.32	108.14	113.80
33	BA	1266	A	N7-C8-N9	-11.32	108.14	113.80
33	BA	1453	A	N7-C8-N9	-11.32	108.14	113.80
33	BA	1724	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	725	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	1463	A	N7-C8-N9	-11.32	108.14	113.80
33	BA	1709	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	929	A	N7-C8-N9	-11.31	108.14	113.80
33	BA	1885	A	N7-C8-N9	-11.31	108.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	622	A	N7-C8-N9	-11.31	108.14	113.80
33	BA	1619	A	N7-C8-N9	-11.31	108.14	113.80
33	BA	339	A	N7-C8-N9	-11.31	108.14	113.80
33	BA	2827	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	875	A	N7-C8-N9	-11.31	108.15	113.80
33	BA	1848	A	N7-C8-N9	-11.31	108.15	113.80
33	BA	2440	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	844	A	N7-C8-N9	-11.30	108.15	113.80
33	BA	1456	A	N7-C8-N9	-11.31	108.15	113.80
33	BA	2869	A	N7-C8-N9	-11.31	108.15	113.80
1	AA	1261	A	N7-C8-N9	-11.30	108.15	113.80
33	BA	118	A	N7-C8-N9	-11.30	108.15	113.80
33	BA	943	A	N7-C8-N9	-11.30	108.15	113.80
33	BA	91	A	N7-C8-N9	-11.30	108.15	113.80
33	BA	275	A	N7-C8-N9	-11.30	108.15	113.80
33	BA	2060	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	1031	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	1128	A	N7-C8-N9	-11.29	108.15	113.80
33	BA	1421	A	N7-C8-N9	-11.29	108.15	113.80
1	AA	1143	A	N7-C8-N9	-11.29	108.16	113.80
33	BA	185	A	N7-C8-N9	-11.29	108.15	113.80
33	BA	623	A	N7-C8-N9	-11.29	108.16	113.80
33	BA	971	A	N7-C8-N9	-11.29	108.15	113.80
33	BA	1388	A	N7-C8-N9	-11.29	108.15	113.80
1	AA	996	A	N7-C8-N9	-11.29	108.16	113.80
33	BA	1361	A	N7-C8-N9	-11.29	108.16	113.80
1	AA	724	A	N7-C8-N9	-11.29	108.16	113.80
33	BA	1074	A	N7-C8-N9	-11.29	108.16	113.80
33	BA	1103	A	N7-C8-N9	-11.29	108.16	113.80
33	BA	1882	A	N7-C8-N9	-11.29	108.16	113.80
33	BA	1888	A	N7-C8-N9	-11.29	108.16	113.80
33	BA	384	A	N7-C8-N9	-11.28	108.16	113.80
1	AA	743	A	N7-C8-N9	-11.28	108.16	113.80
33	BA	178	A	N7-C8-N9	-11.28	108.16	113.80
1	AA	405	A	N3-C4-C5	-11.28	118.91	126.80
33	BA	477	A	N7-C8-N9	-11.28	108.16	113.80
33	BA	1601	A	N7-C8-N9	-11.28	108.16	113.80
33	BA	2463	A	N7-C8-N9	-11.28	108.16	113.80
33	BA	1956	A	N7-C8-N9	-11.28	108.16	113.80
33	BA	560	A	N7-C8-N9	-11.27	108.16	113.80
1	AA	882	A	N7-C8-N9	-11.27	108.16	113.80
1	AA	1179	A	N7-C8-N9	-11.27	108.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	247	A	N7-C8-N9	-11.27	108.17	113.80
33	BA	1221	A	N7-C8-N9	-11.27	108.16	113.80
33	BA	1222	A	N7-C8-N9	-11.27	108.16	113.80
33	BA	1814	A	N7-C8-N9	-11.27	108.17	113.80
33	BA	2205	A	N7-C8-N9	-11.27	108.17	113.80
33	BA	2228	A	N7-C8-N9	-11.27	108.17	113.80
33	BA	2560	A	N7-C8-N9	-11.27	108.17	113.80
33	BA	958	A	N7-C8-N9	-11.27	108.17	113.80
33	BA	1850	A	N7-C8-N9	-11.27	108.17	113.80
33	BA	2441	A	N7-C8-N9	-11.27	108.17	113.80
1	AA	1372	A	N7-C8-N9	-11.27	108.17	113.80
33	BA	2303	A	N7-C8-N9	-11.27	108.17	113.80
1	AA	1283	A	N7-C8-N9	-11.26	108.17	113.80
33	BA	630	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	1297	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	644	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	874	A	N7-C8-N9	-11.26	108.17	113.80
33	BA	1858	A	N7-C8-N9	-11.26	108.17	113.80
33	BA	2831	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	518	A	N7-C8-N9	-11.26	108.17	113.80
33	BA	462	A	N7-C8-N9	-11.26	108.17	113.80
33	BA	661	A	N7-C8-N9	-11.26	108.17	113.80
21	AX	24	A	N7-C8-N9	-11.26	108.17	113.80
1	AA	1272	A	N7-C8-N9	-11.25	108.17	113.80
33	BA	431	A	N7-C8-N9	-11.25	108.17	113.80
33	BA	904	A	N7-C8-N9	-11.25	108.17	113.80
33	BA	2436	A	N7-C8-N9	-11.25	108.17	113.80
33	BA	894	A	N7-C8-N9	-11.25	108.17	113.80
1	AA	758	A	N7-C8-N9	-11.25	108.17	113.80
33	BA	2826	A	N7-C8-N9	-11.25	108.17	113.80
1	AA	209	A	N7-C8-N9	-11.25	108.18	113.80
33	BA	1620	A	N7-C8-N9	-11.25	108.18	113.80
33	BA	2916	A	N7-C8-N9	-11.25	108.18	113.80
33	BA	1905	A	N7-C8-N9	-11.25	108.18	113.80
33	BA	790	A	N7-C8-N9	-11.24	108.18	113.80
1	AA	477	A	N7-C8-N9	-11.24	108.18	113.80
1	AA	711	A	N7-C8-N9	-11.24	108.18	113.80
33	BA	1393	A	N7-C8-N9	-11.24	108.18	113.80
33	BA	56	A	N7-C8-N9	-11.24	108.18	113.80
33	BA	1606	A	N7-C8-N9	-11.24	108.18	113.80
33	BA	2517	A	N7-C8-N9	-11.24	108.18	113.80
1	AA	1166	A	N7-C8-N9	-11.24	108.18	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1697	A	N7-C8-N9	-11.24	108.18	113.80
33	BA	2497	A	N7-C8-N9	-11.24	108.18	113.80
33	BA	391	A	N7-C8-N9	-11.23	108.18	113.80
33	BA	1073	A	N7-C8-N9	-11.23	108.18	113.80
1	AA	1238	A	N7-C8-N9	-11.23	108.18	113.80
33	BA	658	A	N7-C8-N9	-11.23	108.19	113.80
33	BA	925	A	N7-C8-N9	-11.23	108.19	113.80
1	AA	630	A	N7-C8-N9	-11.22	108.19	113.80
33	BA	699	A	N7-C8-N9	-11.22	108.19	113.80
33	BA	52	A	N7-C8-N9	-11.22	108.19	113.80
33	BA	2480	A	N7-C8-N9	-11.22	108.19	113.80
33	BA	268	A	N7-C8-N9	-11.22	108.19	113.80
33	BA	1930	A	N7-C8-N9	-11.22	108.19	113.80
1	AA	713	A	N7-C8-N9	-11.22	108.19	113.80
33	BA	2106	A	N7-C8-N9	-11.22	108.19	113.80
33	BA	2704	A	N7-C8-N9	-11.22	108.19	113.80
1	AA	161	A	N7-C8-N9	-11.21	108.19	113.80
33	BA	2395	A	N7-C8-N9	-11.21	108.19	113.80
34	BB	20	A	N7-C8-N9	-11.21	108.19	113.80
33	BA	61	A	N7-C8-N9	-11.21	108.19	113.80
33	BA	2593	A	N7-C8-N9	-11.21	108.19	113.80
33	BA	1778	A	N7-C8-N9	-11.21	108.20	113.80
33	BA	574	A	N7-C8-N9	-11.21	108.20	113.80
33	BA	2595	A	N7-C8-N9	-11.21	108.20	113.80
33	BA	437	A	N7-C8-N9	-11.21	108.20	113.80
21	AX	23	A	N7-C8-N9	-11.20	108.20	113.80
33	BA	616	A	N7-C8-N9	-11.21	108.20	113.80
1	AA	128	A	N7-C8-N9	-11.20	108.20	113.80
33	BA	38	A	N7-C8-N9	-11.20	108.20	113.80
33	BA	117	A	N7-C8-N9	-11.20	108.20	113.80
33	BA	1945	A	N7-C8-N9	-11.20	108.20	113.80
1	AA	993	A	N3-C4-C5	-11.20	118.96	126.80
33	BA	1714	A	N3-C4-C5	-11.20	118.96	126.80
33	BA	1816	A	N7-C8-N9	-11.20	108.20	113.80
33	BA	2862	A	N7-C8-N9	-11.19	108.20	113.80
33	BA	1614	A	N7-C8-N9	-11.18	108.21	113.80
33	BA	1188	A	N7-C8-N9	-11.18	108.21	113.80
33	BA	1721	A	N7-C8-N9	-11.18	108.21	113.80
33	BA	673	A	N7-C8-N9	-11.18	108.21	113.80
33	BA	1096	A	N7-C8-N9	-11.18	108.21	113.80
33	BA	2111	A	N7-C8-N9	-11.18	108.21	113.80
1	AA	948	A	N7-C8-N9	-11.17	108.21	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	390	A	N7-C8-N9	-11.16	108.22	113.80
33	BA	2044	A	N7-C8-N9	-11.16	108.22	113.80
33	BA	2141	A	N7-C8-N9	-11.16	108.22	113.80
33	BA	2176	A	N7-C8-N9	-11.16	108.22	113.80
1	AA	1161	A	N7-C8-N9	-11.16	108.22	113.80
33	BA	1265	A	N7-C8-N9	-11.16	108.22	113.80
33	BA	1556	A	N7-C8-N9	-11.16	108.22	113.80
34	BB	11	A	N7-C8-N9	-11.16	108.22	113.80
33	BA	956	A	N7-C8-N9	-11.16	108.22	113.80
1	AA	1294	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	1478	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	984	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	74	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	583	A	N7-C8-N9	-11.15	108.22	113.80
33	BA	168	A	N7-C8-N9	-11.15	108.22	113.80
33	BA	2339	A	N7-C8-N9	-11.15	108.23	113.80
33	BA	559	A	N7-C8-N9	-11.15	108.23	113.80
33	BA	2532	A	N7-C8-N9	-11.15	108.23	113.80
1	AA	519	A	N7-C8-N9	-11.14	108.23	113.80
33	BA	2357	A	N7-C8-N9	-11.14	108.23	113.80
33	BA	1767	A	N7-C8-N9	-11.13	108.23	113.80
33	BA	1655	A	N7-C8-N9	-11.13	108.24	113.80
33	BA	95	A	N7-C8-N9	-11.13	108.24	113.80
33	BA	1919	A	N7-C8-N9	-11.12	108.24	113.80
33	BA	2296	A	N7-C8-N9	-11.13	108.24	113.80
21	AX	9	A	N7-C8-N9	-11.12	108.24	113.80
33	BA	2848	A	N7-C8-N9	-11.12	108.24	113.80
33	BA	1480	A	N7-C8-N9	-11.12	108.24	113.80
33	BA	1680	A	N7-C8-N9	-11.11	108.24	113.80
33	BA	343	A	N7-C8-N9	-11.11	108.25	113.80
33	BA	496	A	N7-C8-N9	-11.11	108.25	113.80
33	BA	1244	A	N7-C8-N9	-11.11	108.25	113.80
33	BA	2735	A	N7-C8-N9	-11.10	108.25	113.80
33	BA	2143	A	N7-C8-N9	-11.10	108.25	113.80
1	AA	1366	A	N7-C8-N9	-11.09	108.25	113.80
33	BA	2091	A	N7-C8-N9	-11.09	108.25	113.80
1	AA	99	A	N7-C8-N9	-11.09	108.25	113.80
1	AA	1341	A	N7-C8-N9	-11.09	108.25	113.80
33	BA	689	A	N7-C8-N9	-11.09	108.26	113.80
33	BA	1536	A	N7-C8-N9	-11.09	108.25	113.80
33	BA	948	A	N7-C8-N9	-11.09	108.26	113.80
33	BA	1075	A	N7-C8-N9	-11.09	108.26	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1132	A	N7-C8-N9	-11.09	108.26	113.80
33	BA	2778	A	N7-C8-N9	-11.08	108.26	113.80
34	BB	13	A	N7-C8-N9	-11.08	108.26	113.80
33	BA	494	A	N7-C8-N9	-11.07	108.26	113.80
33	BA	1768	A	N7-C8-N9	-11.07	108.26	113.80
33	BA	527	A	N7-C8-N9	-11.07	108.27	113.80
33	BA	656	A	N7-C8-N9	-11.07	108.27	113.80
33	BA	2252	A	N7-C8-N9	-11.07	108.27	113.80
33	BA	935	A	N3-C4-C5	-11.06	119.06	126.80
33	BA	849	A	N7-C8-N9	-11.06	108.27	113.80
33	BA	1900	A	N7-C8-N9	-11.06	108.27	113.80
33	BA	1360	A	N7-C8-N9	-11.06	108.27	113.80
33	BA	1839	A	N7-C8-N9	-11.05	108.27	113.80
33	BA	1999	A	N7-C8-N9	-11.05	108.27	113.80
33	BA	1832	A	N7-C8-N9	-11.05	108.28	113.80
33	BA	53	A	N7-C8-N9	-11.04	108.28	113.80
33	BA	2123	A	N7-C8-N9	-11.04	108.28	113.80
1	AA	548	A	N7-C8-N9	-11.03	108.28	113.80
1	AA	1155	A	N7-C8-N9	-11.04	108.28	113.80
33	BA	830	A	N7-C8-N9	-11.03	108.28	113.80
33	BA	2164	A	N7-C8-N9	-11.03	108.28	113.80
33	BA	1398	A	N7-C8-N9	-11.03	108.28	113.80
33	BA	2844	A	N7-C8-N9	-11.03	108.28	113.80
1	AA	457	A	N7-C8-N9	-11.03	108.28	113.80
33	BA	1340	A	N7-C8-N9	-11.03	108.28	113.80
33	BA	1506	A	N7-C8-N9	-11.03	108.29	113.80
33	BA	2358	A	N7-C8-N9	-11.03	108.29	113.80
33	BA	2459	A	N7-C8-N9	-11.02	108.29	113.80
33	BA	2468	A	N7-C8-N9	-11.02	108.29	113.80
33	BA	2349	A	N7-C8-N9	-11.02	108.29	113.80
33	BA	1965	A	N7-C8-N9	-11.01	108.29	113.80
33	BA	1562	A	N7-C8-N9	-11.01	108.29	113.80
33	BA	2616	A	N7-C8-N9	-11.01	108.29	113.80
1	AA	969	A	N7-C8-N9	-11.01	108.30	113.80
33	BA	2794	A	N7-C8-N9	-11.00	108.30	113.80
33	BA	1667	A	N7-C8-N9	-11.00	108.30	113.80
34	BB	99	A	N3-C4-C5	-11.00	119.10	126.80
1	AA	1189	A	N7-C8-N9	-10.99	108.31	113.80
33	BA	90	A	N7-C8-N9	-10.99	108.31	113.80
33	BA	1056	A	N7-C8-N9	-10.99	108.31	113.80
33	BA	527	A	N3-C4-C5	-10.99	119.11	126.80
1	AA	1236	A	N7-C8-N9	-10.97	108.31	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1618	A	N7-C8-N9	-10.97	108.31	113.80
1	AA	1315	A	N7-C8-N9	-10.97	108.32	113.80
33	BA	2779	A	N7-C8-N9	-10.96	108.32	113.80
1	AA	405	A	N7-C8-N9	-10.96	108.32	113.80
33	BA	438	A	N7-C8-N9	-10.95	108.32	113.80
33	BA	908	A	N7-C8-N9	-10.95	108.32	113.80
33	BA	1928	A	N7-C8-N9	-10.95	108.32	113.80
1	AA	727	A	N7-C8-N9	-10.95	108.33	113.80
33	BA	1485	A	N7-C8-N9	-10.95	108.33	113.80
33	BA	2407	A	N7-C8-N9	-10.94	108.33	113.80
1	AA	911	A	N7-C8-N9	-10.94	108.33	113.80
33	BA	765	A	N7-C8-N9	-10.94	108.33	113.80
33	BA	913	A	N7-C8-N9	-10.94	108.33	113.80
33	BA	2689	A	N7-C8-N9	-10.92	108.34	113.80
33	BA	1581	A	N3-C4-C5	-10.92	119.16	126.80
1	AA	572	A	N3-C4-C5	-10.91	119.17	126.80
1	AA	1234	A	N7-C8-N9	-10.90	108.35	113.80
33	BA	678	A	N7-C8-N9	-10.90	108.35	113.80
33	BA	1097	A	N7-C8-N9	-10.90	108.35	113.80
33	BA	1774	A	N7-C8-N9	-10.90	108.35	113.80
33	BA	1820	A	N7-C8-N9	-10.90	108.35	113.80
1	AA	1016	A	N7-C8-N9	-10.90	108.35	113.80
1	AA	195	A	N3-C4-C5	-10.89	119.17	126.80
1	AA	1427	A	N7-C8-N9	-10.89	108.36	113.80
1	AA	308	A	N7-C8-N9	-10.89	108.36	113.80
33	BA	2691	A	N7-C8-N9	-10.89	108.36	113.80
33	BA	390	A	N7-C8-N9	-10.87	108.37	113.80
1	AA	439	A	N7-C8-N9	-10.86	108.37	113.80
33	BA	254	A	N7-C8-N9	-10.85	108.37	113.80
33	BA	1877	A	N7-C8-N9	-10.80	108.40	113.80
1	AA	1288	A	N7-C8-N9	-10.80	108.40	113.80
33	BA	1883	A	N7-C8-N9	-10.79	108.40	113.80
33	BA	593	A	N7-C8-N9	-10.79	108.40	113.80
1	AA	555	A	N7-C8-N9	-10.79	108.41	113.80
33	BA	1714	A	N7-C8-N9	-10.79	108.41	113.80
33	BA	513	A	N3-C4-C5	-10.79	119.25	126.80
33	BA	1067	A	N7-C8-N9	-10.79	108.41	113.80
1	AA	987	A	N7-C8-N9	-10.78	108.41	113.80
1	AA	114	A	N7-C8-N9	-10.78	108.41	113.80
1	AA	1234	A	N3-C4-C5	-10.77	119.26	126.80
33	BA	2786	A	N3-C4-C5	-10.77	119.26	126.80
33	BA	913	A	N3-C4-C5	-10.77	119.26	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1491	A	N7-C8-N9	-10.76	108.42	113.80
33	BA	634	A	N7-C8-N9	-10.73	108.44	113.80
1	AA	391	A	N7-C8-N9	-10.72	108.44	113.80
1	AA	195	A	N7-C8-N9	-10.71	108.44	113.80
1	AA	572	A	N7-C8-N9	-10.71	108.44	113.80
1	AA	1288	A	N3-C4-C5	-10.67	119.33	126.80
1	AA	1026	A	N7-C8-N9	-10.66	108.47	113.80
33	BA	593	A	N3-C4-C5	-10.65	119.34	126.80
1	AA	933	A	N7-C8-N9	-10.64	108.48	113.80
33	BA	2202	A	N3-C4-C5	-10.62	119.36	126.80
33	BA	390	A	N3-C4-C5	-10.60	119.38	126.80
1	AA	99	A	N3-C4-C5	-10.60	119.38	126.80
33	BA	1019	A	N7-C8-N9	-10.57	108.51	113.80
33	BA	2885	A	N7-C8-N9	-10.56	108.52	113.80
1	AA	1026	A	N3-C4-C5	-10.55	119.41	126.80
33	BA	1581	A	N7-C8-N9	-10.54	108.53	113.80
33	BA	2202	A	N7-C8-N9	-10.54	108.53	113.80
33	BA	935	A	N7-C8-N9	-10.53	108.53	113.80
33	BA	2786	A	N7-C8-N9	-10.53	108.54	113.80
1	AA	987	A	N3-C4-C5	-10.52	119.44	126.80
33	BA	254	A	N3-C4-C5	-10.51	119.44	126.80
33	BA	1667	A	N3-C4-C5	-10.51	119.44	126.80
33	BA	2143	A	N3-C4-C5	-10.50	119.45	126.80
1	AA	1341	A	N3-C4-C5	-10.49	119.45	126.80
33	BA	1006	A	N3-C4-C5	-10.49	119.46	126.80
33	BA	2627	A	N7-C8-N9	-10.48	108.56	113.80
1	AA	1308	A	N7-C8-N9	-10.47	108.56	113.80
33	BA	1562	A	N3-C4-C5	-10.46	119.48	126.80
33	BA	948	A	N3-C4-C5	-10.44	119.50	126.80
33	BA	2627	A	N3-C4-C5	-10.44	119.50	126.80
33	BA	736	A	N3-C4-C5	-10.43	119.50	126.80
33	BA	2459	A	N3-C4-C5	-10.43	119.50	126.80
33	BA	2794	A	N3-C4-C5	-10.43	119.50	126.80
33	BA	732	A	N3-C4-C5	-10.42	119.50	126.80
33	BA	1006	A	N7-C8-N9	-10.41	108.59	113.80
33	BA	2885	A	N3-C4-C5	-10.41	119.51	126.80
33	BA	2844	A	N3-C4-C5	-10.40	119.52	126.80
33	BA	2735	A	N3-C4-C5	-10.40	119.52	126.80
33	BA	1360	A	N3-C4-C5	-10.39	119.52	126.80
33	BA	1073	A	N3-C4-C5	-10.38	119.54	126.80
33	BA	1480	A	N3-C4-C5	-10.37	119.54	126.80
1	AA	114	A	N3-C4-C5	-10.37	119.54	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1491	A	N3-C4-C5	-10.36	119.55	126.80
1	AA	727	A	N3-C4-C5	-10.35	119.55	126.80
1	AA	1278	A	N7-C8-N9	-10.35	108.62	113.80
33	BA	1778	A	N3-C4-C5	-10.35	119.55	126.80
33	BA	679	A	N7-C8-N9	-10.35	108.63	113.80
33	BA	2339	A	N3-C4-C5	-10.35	119.56	126.80
33	BA	1485	A	N3-C4-C5	-10.34	119.56	126.80
33	BA	634	A	N3-C4-C5	-10.34	119.56	126.80
33	BA	679	A	N3-C4-C5	-10.34	119.56	126.80
1	AA	308	A	N3-C4-C5	-10.33	119.57	126.80
34	BB	11	A	N3-C4-C5	-10.33	119.57	126.80
33	BA	185	A	N3-C4-C5	-10.33	119.57	126.80
33	BA	551	A	N3-C4-C5	-10.32	119.57	126.80
33	BA	2407	A	N3-C4-C5	-10.32	119.57	126.80
1	AA	993	A	N7-C8-N9	-10.32	108.64	113.80
1	AA	391	A	N3-C4-C5	-10.31	119.58	126.80
33	BA	732	A	N7-C8-N9	-10.31	108.64	113.80
33	BA	365	U	P-O3'-C3'	-10.31	107.33	119.70
33	BA	108	A	N3-C4-C5	-10.30	119.59	126.80
33	BA	2532	A	N3-C4-C5	-10.30	119.59	126.80
33	BA	2689	A	N3-C4-C5	-10.29	119.59	126.80
1	AA	397	A	N3-C4-C5	-10.29	119.59	126.80
1	AA	1278	A	N3-C4-C5	-10.29	119.60	126.80
33	BA	1877	A	N3-C4-C5	-10.29	119.59	126.80
1	AA	1166	A	N3-C4-C5	-10.29	119.60	126.80
1	AA	933	A	N3-C4-C5	-10.29	119.60	126.80
33	BA	1019	A	N3-C4-C5	-10.29	119.60	126.80
33	BA	1506	A	N3-C4-C5	-10.29	119.60	126.80
33	BA	438	A	N3-C4-C5	-10.28	119.60	126.80
33	BA	1398	A	N3-C4-C5	-10.27	119.61	126.80
33	BA	226	A	N7-C8-N9	-10.27	108.67	113.80
33	BA	2123	A	N3-C4-C5	-10.27	119.61	126.80
33	BA	2691	A	N3-C4-C5	-10.27	119.61	126.80
1	AA	649	A	N3-C4-C5	-10.26	119.61	126.80
33	BA	715	A	N3-C4-C5	-10.25	119.62	126.80
33	BA	1900	A	N3-C4-C5	-10.25	119.63	126.80
1	AA	844	A	N3-C4-C5	-10.24	119.63	126.80
33	BA	656	A	N3-C4-C5	-10.24	119.63	126.80
33	BA	1096	A	N3-C4-C5	-10.24	119.63	126.80
33	BA	1536	A	N3-C4-C5	-10.24	119.63	126.80
1	AA	1427	A	N3-C4-C5	-10.24	119.63	126.80
33	BA	437	A	N3-C4-C5	-10.24	119.63	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2402	A	N3-C4-C5	-10.23	119.64	126.80
1	AA	507	A	N3-C4-C5	-10.23	119.64	126.80
33	BA	2862	A	N3-C4-C5	-10.23	119.64	126.80
33	BA	1691	A	N7-C8-N9	-10.22	108.69	113.80
33	BA	2176	A	N3-C4-C5	-10.22	119.64	126.80
33	BA	1816	A	N3-C4-C5	-10.22	119.65	126.80
1	AA	128	A	N3-C4-C5	-10.21	119.65	126.80
33	BA	1103	A	N3-C4-C5	-10.21	119.65	126.80
33	BA	689	A	N3-C4-C5	-10.21	119.65	126.80
33	BA	56	A	N3-C4-C5	-10.21	119.65	126.80
33	BA	1132	A	N3-C4-C5	-10.21	119.65	126.80
33	BA	2106	A	N3-C4-C5	-10.20	119.66	126.80
33	BA	1638	A	N3-C4-C5	-10.20	119.66	126.80
33	BA	1442	A	N3-C4-C5	-10.20	119.66	126.80
33	BA	1858	A	N3-C4-C5	-10.20	119.66	126.80
33	BA	2205	A	N3-C4-C5	-10.20	119.66	126.80
33	BA	1710	A	N3-C4-C5	-10.20	119.66	126.80
34	BB	13	A	N3-C4-C5	-10.20	119.66	126.80
1	AA	1155	A	N3-C4-C5	-10.19	119.66	126.80
33	BA	559	A	N3-C4-C5	-10.19	119.66	126.80
33	BA	1618	A	N3-C4-C5	-10.19	119.66	126.80
33	BA	2111	A	N3-C4-C5	-10.19	119.67	126.80
33	BA	1392	A	N3-C4-C5	-10.19	119.67	126.80
33	BA	95	A	N3-C4-C5	-10.19	119.67	126.80
33	BA	1999	A	N3-C4-C5	-10.19	119.67	126.80
1	AA	1315	A	N3-C4-C5	-10.18	119.67	126.80
33	BA	2117	A	N3-C4-C5	-10.18	119.67	126.80
33	BA	2436	A	N3-C4-C5	-10.18	119.68	126.80
33	BA	2329	A	N3-C4-C5	-10.18	119.68	126.80
33	BA	765	A	N3-C4-C5	-10.17	119.68	126.80
33	BA	2349	A	N3-C4-C5	-10.17	119.68	126.80
1	AA	1143	A	N3-C4-C5	-10.17	119.68	126.80
34	BB	46	A	N3-C4-C5	-10.17	119.68	126.80
21	AX	24	A	N3-C4-C5	-10.16	119.69	126.80
33	BA	130	A	N3-C4-C5	-10.16	119.69	126.80
1	AA	74	A	N3-C4-C5	-10.16	119.69	126.80
33	BA	560	A	N3-C4-C5	-10.16	119.69	126.80
33	BA	1490	A	N3-C4-C5	-10.16	119.69	126.80
1	AA	1160	A	N3-C4-C5	-10.16	119.69	126.80
33	BA	574	A	N3-C4-C5	-10.16	119.69	126.80
33	BA	2351	A	N3-C4-C5	-10.16	119.69	126.80
33	BA	910	A	N3-C4-C5	-10.15	119.70	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	956	A	N3-C4-C5	-10.14	119.70	126.80
21	AX	9	A	N3-C4-C5	-10.14	119.70	126.80
33	BA	1653	A	N3-C4-C5	-10.14	119.70	126.80
33	BA	1258	A	N3-C4-C5	-10.14	119.70	126.80
33	BA	2043	A	N3-C4-C5	-10.13	119.70	126.80
33	BA	1222	A	N3-C4-C5	-10.13	119.71	126.80
33	BA	1046	A	N3-C4-C5	-10.13	119.71	126.80
33	BA	52	A	N3-C4-C5	-10.13	119.71	126.80
1	AA	282	A	N3-C4-C5	-10.13	119.71	126.80
33	BA	866	A	N3-C4-C5	-10.13	119.71	126.80
33	BA	2790	A	N3-C4-C5	-10.12	119.71	126.80
33	BA	849	A	N3-C4-C5	-10.12	119.72	126.80
1	AA	790	A	N3-C4-C5	-10.12	119.72	126.80
33	BA	44	A	N3-C4-C5	-10.12	119.72	126.80
33	BA	673	A	N3-C4-C5	-10.12	119.72	126.80
33	BA	1885	A	N3-C4-C5	-10.12	119.72	126.80
33	BA	2358	A	N3-C4-C5	-10.12	119.72	126.80
33	BA	2049	A	N3-C4-C5	-10.11	119.72	126.80
33	BA	2027	A	N3-C4-C5	-10.11	119.72	126.80
33	BA	407	A	N3-C4-C5	-10.11	119.72	126.80
33	BA	2812	A	N3-C4-C5	-10.11	119.72	126.80
1	AA	721	A	N3-C4-C5	-10.11	119.73	126.80
33	BA	970	A	N3-C4-C5	-10.11	119.73	126.80
33	BA	2026	A	N3-C4-C5	-10.10	119.73	126.80
33	BA	168	A	N3-C4-C5	-10.10	119.73	126.80
1	AA	337	A	N3-C4-C5	-10.10	119.73	126.80
33	BA	353	A	N3-C4-C5	-10.10	119.73	126.80
33	BA	943	A	N3-C4-C5	-10.10	119.73	126.80
33	BA	1839	A	N3-C4-C5	-10.10	119.73	126.80
1	AA	948	A	N3-C4-C5	-10.10	119.73	126.80
1	AA	1065	A	N3-C4-C5	-10.10	119.73	126.80
33	BA	2662	A	N3-C4-C5	-10.10	119.73	126.80
33	BA	2395	A	N3-C4-C5	-10.10	119.73	126.80
1	AA	57	A	N3-C4-C5	-10.09	119.74	126.80
1	AA	1272	A	N3-C4-C5	-10.09	119.73	126.80
33	BA	265	A	N3-C4-C5	-10.09	119.73	126.80
33	BA	513	A	N7-C8-N9	-10.09	108.75	113.80
33	BA	925	A	N3-C4-C5	-10.09	119.73	126.80
33	BA	1094	A	N3-C4-C5	-10.09	119.73	126.80
33	BA	1393	A	N3-C4-C5	-10.09	119.74	126.80
1	AA	555	A	N3-C4-C5	-10.09	119.74	126.80
33	BA	2163	A	N3-C4-C5	-10.09	119.74	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	838	A	N3-C4-C5	-10.08	119.74	126.80
33	BA	1286	A	N3-C4-C5	-10.08	119.74	126.80
33	BA	1005	A	N3-C4-C5	-10.08	119.74	126.80
33	BA	1075	A	N3-C4-C5	-10.08	119.74	126.80
33	BA	1883	A	N3-C4-C5	-10.08	119.75	126.80
33	BA	1709	A	N3-C4-C5	-10.07	119.75	126.80
33	BA	2343	A	N3-C4-C5	-10.07	119.75	126.80
33	BA	1190	A	N3-C4-C5	-10.07	119.75	126.80
33	BA	38	A	N3-C4-C5	-10.06	119.75	126.80
33	BA	690	A	N3-C4-C5	-10.06	119.75	126.80
33	BA	2044	A	N3-C4-C5	-10.06	119.75	126.80
1	AA	55	A	N3-C4-C5	-10.06	119.76	126.80
33	BA	133	A	N3-C4-C5	-10.06	119.76	126.80
33	BA	1831	A	N3-C4-C5	-10.06	119.76	126.80
1	AA	630	A	N3-C4-C5	-10.06	119.76	126.80
33	BA	496	A	N3-C4-C5	-10.06	119.76	126.80
33	BA	1655	A	N3-C4-C5	-10.06	119.76	126.80
33	BA	2848	A	N3-C4-C5	-10.06	119.76	126.80
1	AA	1004	A	N3-C4-C5	-10.06	119.76	126.80
34	BB	71	A	N3-C4-C5	-10.06	119.76	126.80
33	BA	2722	A	N3-C4-C5	-10.06	119.76	126.80
33	BA	1235	A	N3-C4-C5	-10.05	119.76	126.80
33	BA	2826	A	N3-C4-C5	-10.05	119.76	126.80
33	BA	2100	A	N3-C4-C5	-10.05	119.77	126.80
1	AA	911	A	N3-C4-C5	-10.05	119.77	126.80
1	AA	711	A	N3-C4-C5	-10.04	119.77	126.80
33	BA	326	A	N3-C4-C5	-10.04	119.77	126.80
33	BA	1316	A	N3-C4-C5	-10.04	119.77	126.80
33	BA	518	A	N3-C4-C5	-10.04	119.77	126.80
33	BA	592	A	N3-C4-C5	-10.04	119.77	126.80
33	BA	661	A	N3-C4-C5	-10.04	119.77	126.80
33	BA	2831	A	N3-C4-C5	-10.04	119.77	126.80
1	AA	72	A	N3-C4-C5	-10.03	119.78	126.80
1	AA	1384	A	N3-C4-C5	-10.03	119.78	126.80
33	BA	752	A	N3-C4-C5	-10.03	119.78	126.80
33	BA	1524	A	N3-C4-C5	-10.03	119.78	126.80
33	BA	1776	A	N3-C4-C5	-10.03	119.78	126.80
1	AA	945	A	N3-C4-C5	-10.03	119.78	126.80
33	BA	391	A	N3-C4-C5	-10.03	119.78	126.80
33	BA	1426	A	N3-C4-C5	-10.03	119.78	126.80
33	BA	957	A	N3-C4-C5	-10.03	119.78	126.80
33	BA	1357	A	N3-C4-C5	-10.03	119.78	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	76	A	N3-C4-C5	-10.03	119.78	126.80
33	BA	1614	A	N3-C4-C5	-10.03	119.78	126.80
33	BA	2500	A	N3-C4-C5	-10.03	119.78	126.80
33	BA	724	A	N3-C4-C5	-10.02	119.78	126.80
33	BA	2560	A	N3-C4-C5	-10.02	119.78	126.80
1	AA	1442	A	N3-C4-C5	-10.02	119.78	126.80
33	BA	1126	A	N3-C4-C5	-10.02	119.78	126.80
1	AA	617	A	N3-C4-C5	-10.02	119.79	126.80
1	AA	1369	A	N3-C4-C5	-10.02	119.79	126.80
33	BA	896	A	N3-C4-C5	-10.02	119.79	126.80
33	BA	2517	A	N3-C4-C5	-10.02	119.79	126.80
34	BB	97	A	N3-C4-C5	-10.02	119.79	126.80
1	AA	996	A	N3-C4-C5	-10.02	119.79	126.80
33	BA	1619	A	N3-C4-C5	-10.02	119.79	126.80
1	AA	1517	A	N3-C4-C5	-10.02	119.79	126.80
33	BA	456	A	N3-C4-C5	-10.02	119.79	126.80
33	BA	1820	A	N3-C4-C5	-10.02	119.79	126.80
33	BA	889	A	N3-C4-C5	-10.01	119.79	126.80
33	BA	974	A	N3-C4-C5	-10.01	119.79	126.80
21	AX	70	A	N3-C4-C5	-10.01	119.79	126.80
1	AA	758	A	N3-C4-C5	-10.01	119.80	126.80
1	AA	1256	A	N3-C4-C5	-10.01	119.79	126.80
1	AA	1349	A	N3-C4-C5	-10.01	119.79	126.80
1	AA	1179	A	N3-C4-C5	-10.01	119.80	126.80
1	AA	1189	A	N3-C4-C5	-10.01	119.80	126.80
33	BA	258	A	N3-C4-C5	-10.01	119.80	126.80
33	BA	530	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	743	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	1112	A	N3-C4-C5	-10.00	119.80	126.80
33	BA	2700	A	N3-C4-C5	-10.00	119.80	126.80
33	BA	2924	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	1435	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	1016	A	N3-C4-C5	-10.00	119.80	126.80
33	BA	1672	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	1236	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	1490	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	140	A	N3-C4-C5	-9.99	119.80	126.80
33	BA	956	A	N3-C4-C5	-9.99	119.80	126.80
1	AA	715	A	N3-C4-C5	-9.99	119.81	126.80
33	BA	549	A	N3-C4-C5	-9.99	119.81	126.80
33	BA	61	A	N3-C4-C5	-9.99	119.81	126.80
33	BA	90	A	N3-C4-C5	-9.99	119.81	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2164	A	N3-C4-C5	-9.99	119.81	126.80
33	BA	538	A	N3-C4-C5	-9.99	119.81	126.80
33	BA	952	A	N3-C4-C5	-9.99	119.81	126.80
1	AA	605	A	N3-C4-C5	-9.98	119.81	126.80
33	BA	1695	A	N3-C4-C5	-9.98	119.81	126.80
33	BA	2270	A	N3-C4-C5	-9.98	119.81	126.80
33	BA	2663	A	N3-C4-C5	-9.98	119.81	126.80
1	AA	301	A	N3-C4-C5	-9.98	119.81	126.80
33	BA	500	A	N3-C4-C5	-9.98	119.81	126.80
33	BA	870	A	N3-C4-C5	-9.98	119.81	126.80
1	AA	984	A	N3-C4-C5	-9.98	119.81	126.80
33	BA	578	A	N3-C4-C5	-9.98	119.81	126.80
1	AA	671	A	N3-C4-C5	-9.98	119.81	126.80
1	AA	793	A	N3-C4-C5	-9.98	119.82	126.80
33	BA	462	A	N3-C4-C5	-9.98	119.81	126.80
33	BA	2754	A	N3-C4-C5	-9.98	119.81	126.80
1	AA	1178	A	N3-C4-C5	-9.98	119.82	126.80
33	BA	2052	A	N3-C4-C5	-9.98	119.82	126.80
1	AA	433	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	281	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	429	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	1425	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	193	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	2629	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	722	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	2220	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	2252	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	2547	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	2369	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	548	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	1945	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	404	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	1478	A	N3-C4-C5	-9.97	119.82	126.80
33	BA	1768	A	N3-C4-C5	-9.96	119.82	126.80
33	BA	2302	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	1029	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	1483	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	1956	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	517	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	616	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	1074	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	875	A	N3-C4-C5	-9.96	119.83	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	882	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	171	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	1493	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	692	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	1388	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	918	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	790	A	N3-C4-C5	-9.96	119.83	126.80
33	BA	1636	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	129	A	N3-C4-C5	-9.95	119.83	126.80
33	BA	882	A	N3-C4-C5	-9.95	119.83	126.80
1	AA	512	A	N3-C4-C5	-9.95	119.83	126.80
33	BA	1260	A	N3-C4-C5	-9.95	119.84	126.80
33	BA	1421	A	N3-C4-C5	-9.95	119.84	126.80
33	BA	2694	A	N3-C4-C5	-9.95	119.84	126.80
33	BA	431	A	N3-C4-C5	-9.95	119.84	126.80
33	BA	2900	A	N3-C4-C5	-9.95	119.84	126.80
33	BA	1210	A	N3-C4-C5	-9.94	119.84	126.80
33	BA	678	A	N3-C4-C5	-9.94	119.84	126.80
33	BA	1100	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	659	A	N3-C4-C5	-9.94	119.84	126.80
33	BA	1888	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	335	A	N3-C4-C5	-9.94	119.84	126.80
33	BA	156	A	N3-C4-C5	-9.94	119.85	126.80
33	BA	486	A	N3-C4-C5	-9.94	119.84	126.80
33	BA	2047	A	N3-C4-C5	-9.94	119.84	126.80
33	BA	206	A	N3-C4-C5	-9.93	119.85	126.80
33	BA	894	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	1320	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	913	A	N3-C4-C5	-9.93	119.85	126.80
33	BA	1556	A	N3-C4-C5	-9.93	119.85	126.80
33	BA	318	A	N3-C4-C5	-9.93	119.85	126.80
33	BA	1174	A	N3-C4-C5	-9.93	119.85	126.80
33	BA	1194	A	N3-C4-C5	-9.92	119.85	126.80
1	AA	364	A	N3-C4-C5	-9.92	119.86	126.80
1	AA	1486	A	N3-C4-C5	-9.92	119.85	126.80
33	BA	21	A	N3-C4-C5	-9.92	119.85	126.80
33	BA	1845	A	N3-C4-C5	-9.92	119.85	126.80
33	BA	2091	A	N3-C4-C5	-9.92	119.85	126.80
1	AA	270	A	N3-C4-C5	-9.92	119.86	126.80
33	BA	2066	A	N3-C4-C5	-9.92	119.86	126.80
33	BA	1727	A	N3-C4-C5	-9.92	119.86	126.80
33	BA	384	A	N3-C4-C5	-9.92	119.86	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2200	A	N3-C4-C5	-9.92	119.86	126.80
33	BA	2511	A	N3-C4-C5	-9.92	119.86	126.80
33	BA	2805	A	N3-C4-C5	-9.92	119.86	126.80
33	BA	2827	A	N3-C4-C5	-9.92	119.86	126.80
1	AA	173	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	758	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	1253	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	1265	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	1617	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	2779	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	652	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	1685	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	2854	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	275	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	1620	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	2616	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	2846	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	278	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	469	A	N3-C4-C5	-9.91	119.86	126.80
33	BA	1243	A	N3-C4-C5	-9.91	119.87	126.80
33	BA	1700	A	N3-C4-C5	-9.91	119.87	126.80
33	BA	279	A	N3-C4-C5	-9.90	119.87	126.80
33	BA	2441	A	N3-C4-C5	-9.90	119.87	126.80
33	BA	2830	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	811	A	N3-C4-C5	-9.90	119.87	126.80
21	AX	41	A	N3-C4-C5	-9.90	119.87	126.80
33	BA	12	A	N3-C4-C5	-9.90	119.87	126.80
33	BA	140	A	N3-C4-C5	-9.90	119.87	126.80
33	BA	1760	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	61	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	161	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	1297	A	N3-C4-C5	-9.90	119.87	126.80
33	BA	259	A	N3-C4-C5	-9.90	119.87	126.80
33	BA	1008	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	234	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	278	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	959	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	1222	A	N3-C4-C5	-9.90	119.87	126.80
33	BA	230	A	N3-C4-C5	-9.90	119.87	126.80
21	AX	23	A	N3-C4-C5	-9.89	119.87	126.80
33	BA	41	A	N3-C4-C5	-9.89	119.87	126.80
1	AA	658	A	N3-C4-C5	-9.89	119.88	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	978	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	6	A	N3-C4-C5	-9.89	119.87	126.80
33	BA	922	A	N3-C4-C5	-9.89	119.87	126.80
33	BA	1424	A	N3-C4-C5	-9.89	119.87	126.80
33	BA	1895	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	2834	A	N3-C4-C5	-9.89	119.87	126.80
33	BA	2919	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	139	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	917	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	1327	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	883	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	1260	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	305	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	2464	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	1405	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	1575	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	2769	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	507	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	1461	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	1876	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	2902	A	N3-C4-C5	-9.89	119.88	126.80
34	BB	50	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	462	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	1206	A	N3-C4-C5	-9.89	119.88	126.80
33	BA	1998	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	968	A	N3-C4-C5	-9.88	119.88	126.80
33	BA	1995	A	N3-C4-C5	-9.88	119.88	126.80
33	BA	2845	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	477	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	518	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	928	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	1359	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	1463	A	N3-C4-C5	-9.88	119.88	126.80
33	BA	376	A	N3-C4-C5	-9.88	119.88	126.80
33	BA	173	A	N3-C4-C5	-9.88	119.88	126.80
33	BA	1774	A	N3-C4-C5	-9.88	119.88	126.80
1	AA	796	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	1383	A	N3-C4-C5	-9.88	119.89	126.80
33	BA	1680	A	N3-C4-C5	-9.88	119.89	126.80
33	BA	2570	A	N3-C4-C5	-9.88	119.89	126.80
33	BA	2590	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	225	A	N3-C4-C5	-9.88	119.89	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1283	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	1523	A	N3-C4-C5	-9.88	119.89	126.80
33	BA	1981	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	2365	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	390	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	1024	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	630	A	N3-C4-C5	-9.87	119.89	126.80
34	BB	18	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	506	A	N3-C4-C5	-9.87	119.89	126.80
21	AX	14	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	2907	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	1238	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	964	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	971	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	1542	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	1366	A	N3-C4-C5	-9.87	119.89	126.80
21	AX	21	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	102	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	699	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	2080	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	2148	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	2228	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	2619	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	2704	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	2889	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	1027	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	346	A	N3-C4-C5	-9.86	119.89	126.80
1	AA	1455	A	N3-C4-C5	-9.86	119.89	126.80
33	BA	623	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	1056	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	1520	A	N3-C4-C5	-9.86	119.89	126.80
33	BA	1569	A	N3-C4-C5	-9.87	119.89	126.80
33	BA	1745	A	N3-C4-C5	-9.86	119.89	126.80
33	BA	1965	A	N3-C4-C5	-9.86	119.89	126.80
1	AA	902	A	N3-C4-C5	-9.86	119.90	126.80
21	AX	44	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	1686	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	824	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	1055	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	73	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	1059	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	2165	A	N3-C4-C5	-9.86	119.90	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2227	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	52	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	452	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	117	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	870	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	1437	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	231	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	1097	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	1838	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	1848	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	1882	A	N3-C4-C5	-9.86	119.90	126.80
33	BA	2668	A	N3-C4-C5	-9.86	119.90	126.80
1	AA	669	A	N3-C4-C5	-9.85	119.90	126.80
1	AA	1022	A	N3-C4-C5	-9.85	119.90	126.80
33	BA	867	A	N3-C4-C5	-9.85	119.90	126.80
33	BA	769	A	N3-C4-C5	-9.85	119.90	126.80
33	BA	1675	A	N3-C4-C5	-9.85	119.90	126.80
33	BA	2042	A	N3-C4-C5	-9.85	119.90	126.80
33	BA	1928	A	N3-C4-C5	-9.85	119.90	126.80
33	BA	2461	A	N3-C4-C5	-9.85	119.90	126.80
1	AA	382	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	496	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	886	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	919	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	1348	A	N3-C4-C5	-9.85	119.91	126.80
33	BA	1477	A	N3-C4-C5	-9.85	119.91	126.80
33	BA	753	A	N3-C4-C5	-9.85	119.91	126.80
33	BA	1445	A	N3-C4-C5	-9.85	119.91	126.80
33	BA	1541	A	N3-C4-C5	-9.85	119.91	126.80
21	AX	58	A	N3-C4-C5	-9.85	119.91	126.80
33	BA	449	A	N3-C4-C5	-9.85	119.91	126.80
33	BA	1532	A	N3-C4-C5	-9.85	119.91	126.80
33	BA	1663	A	N3-C4-C5	-9.85	119.91	126.80
33	BA	2497	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	768	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	91	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	705	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1284	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	144	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	329	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	637	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	1284	A	N3-C4-C5	-9.84	119.91	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1631	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	34	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	459	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1092	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	178	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	307	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	330	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	1583	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	2078	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	705	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	1197	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	1346	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	2327	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	2357	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	2389	A	N3-C4-C5	-9.84	119.91	126.80
33	BA	2643	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	81	A	N3-C4-C5	-9.84	119.92	126.80
1	AA	1509	A	N3-C4-C5	-9.84	119.92	126.80
33	BA	459	A	N3-C4-C5	-9.84	119.92	126.80
33	BA	1233	A	N3-C4-C5	-9.84	119.92	126.80
33	BA	2170	A	N3-C4-C5	-9.84	119.92	126.80
33	BA	2462	A	N3-C4-C5	-9.84	119.92	126.80
1	AA	12	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	677	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	2316	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	664	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	1245	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	220	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	2119	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	2887	A	N3-C4-C5	-9.83	119.92	126.80
21	AX	76	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	268	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	851	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	1832	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	124	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	260	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	1767	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	2317	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	314	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	737	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	475	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	771	A	N3-C4-C5	-9.83	119.92	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	803	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	1147	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	194	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	1947	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	548	A	N3-C4-C5	-9.83	119.92	126.80
33	BA	1697	A	N3-C4-C5	-9.83	119.92	126.80
34	BB	64	A	N3-C4-C5	-9.83	119.92	126.80
1	AA	529	A	N3-C4-C5	-9.82	119.92	126.80
1	AA	1128	A	N3-C4-C5	-9.82	119.92	126.80
33	BA	2505	A	N3-C4-C5	-9.82	119.92	126.80
33	BA	908	A	N3-C4-C5	-9.82	119.92	126.80
33	BA	1585	A	N3-C4-C5	-9.82	119.92	126.80
33	BA	2869	A	N3-C4-C5	-9.82	119.92	126.80
33	BA	1627	A	N3-C4-C5	-9.82	119.92	126.80
33	BA	2406	A	N3-C4-C5	-9.82	119.92	126.80
1	AA	361	A	N3-C4-C5	-9.82	119.92	126.80
1	AA	672	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	1115	A	N3-C4-C5	-9.82	119.92	126.80
33	BA	2468	A	N3-C4-C5	-9.82	119.92	126.80
1	AA	1121	A	N3-C4-C5	-9.82	119.93	126.80
33	BA	222	A	N3-C4-C5	-9.82	119.93	126.80
33	BA	412	A	N3-C4-C5	-9.82	119.93	126.80
33	BA	1608	A	N3-C4-C5	-9.82	119.93	126.80
33	BA	2146	A	N3-C4-C5	-9.82	119.92	126.80
33	BA	2338	A	N3-C4-C5	-9.82	119.92	126.80
33	BA	2381	A	N3-C4-C5	-9.82	119.93	126.80
33	BA	2762	A	N3-C4-C5	-9.82	119.92	126.80
34	BB	51	A	N3-C4-C5	-9.82	119.93	126.80
34	BB	99	A	N7-C8-N9	-9.82	108.89	113.80
1	AA	371	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	522	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	1180	A	N3-C4-C5	-9.82	119.93	126.80
33	BA	369	A	N3-C4-C5	-9.82	119.93	126.80
33	BA	1580	A	N3-C4-C5	-9.82	119.93	126.80
34	BB	20	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	381	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	1014	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	1252	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	1028	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	1161	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	200	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1930	A	N3-C4-C5	-9.81	119.93	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2141	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	2216	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	251	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	801	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	343	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	762	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	987	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1025	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1588	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1788	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1989	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	604	A	N3-C4-C5	-9.81	119.94	126.80
33	BA	770	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1047	A	N3-C4-C5	-9.81	119.94	126.80
33	BA	1254	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1269	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1312	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1423	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1724	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	2750	A	N3-C4-C5	-9.81	119.93	126.80
33	BA	1723	A	N3-C4-C5	-9.81	119.94	126.80
33	BA	2593	A	N3-C4-C5	-9.81	119.94	126.80
1	AA	1213	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	519	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	1593	A	N3-C4-C5	-9.81	119.94	126.80
33	BA	2477	A	N3-C4-C5	-9.81	119.94	126.80
33	BA	958	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	2087	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	2152	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	2734	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	2356	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	2782	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	2837	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	696	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1259	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	225	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	337	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	1361	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	1925	A	N3-C4-C5	-9.80	119.94	126.80
34	BB	114	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	372	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	685	A	N3-C4-C5	-9.80	119.94	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	679	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1270	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	65	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	622	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	978	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	2303	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	2447	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	190	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	271	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	1298	A	N3-C4-C5	-9.79	119.94	126.80
33	BA	10	A	N3-C4-C5	-9.79	119.94	126.80
33	BA	537	A	N3-C4-C5	-9.79	119.94	126.80
33	BA	543	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	868	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	1516	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	2000	A	N3-C4-C5	-9.80	119.94	126.80
33	BA	2034	A	N3-C4-C5	-9.79	119.94	126.80
1	AA	287	A	N3-C4-C5	-9.79	119.94	126.80
1	AA	828	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	1140	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	524	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	1113	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	2661	A	N3-C4-C5	-9.79	119.95	126.80
34	BB	76	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	725	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	874	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	428	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	2124	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	2498	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	762	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	436	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	1615	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	479	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	1918	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	35	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	1403	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	364	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	1054	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	1157	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	1230	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	1592	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	388	A	N3-C4-C5	-9.78	119.95	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	470	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	1381	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	1404	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	1406	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	2060	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	2571	A	N3-C4-C5	-9.79	119.95	126.80
33	BA	2787	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	389	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	1502	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	888	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	2719	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	979	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	658	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	830	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	1130	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	1677	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	1721	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	2658	A	N3-C4-C5	-9.78	119.95	126.80
34	BB	105	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	1813	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	423	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	440	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	1054	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	5	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	1277	A	N3-C4-C5	-9.78	119.96	126.80
33	BA	1323	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	2440	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	1375	A	N3-C4-C5	-9.78	119.95	126.80
33	BA	2904	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	94	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	504	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	1271	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	1342	A	N3-C4-C5	-9.78	119.96	126.80
33	BA	333	A	N3-C4-C5	-9.78	119.96	126.80
33	BA	2387	A	N3-C4-C5	-9.78	119.96	126.80
33	BA	2778	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	240	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	491	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	53	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	808	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	1313	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	1961	A	N3-C4-C5	-9.77	119.96	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2421	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	344	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	1185	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	876	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	2298	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	2307	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	373	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	2006	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	170	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	1103	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	339	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	2454	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	2740	A	N3-C4-C5	-9.77	119.96	126.80
34	BB	56	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	1111	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	893	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	965	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	1144	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	1746	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	1789	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	1901	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	2018	A	N3-C4-C5	-9.77	119.96	126.80
33	BA	14	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	94	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	110	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	561	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	2083	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	439	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	485	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	236	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	281	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	786	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	418	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	1200	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	1456	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	1529	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	600	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	1735	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	2463	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	2893	A	N3-C4-C5	-9.76	119.97	126.80
34	BB	27	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	947	A	N3-C4-C5	-9.76	119.97	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1797	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	592	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	650	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	1513	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	13	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	547	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	1026	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	1405	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	1464	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	1534	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	2030	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	2256	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	2405	A	N3-C4-C5	-9.76	119.97	126.80
33	BA	2686	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	1031	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	1120	A	N3-C4-C5	-9.75	119.97	126.80
33	BA	216	A	N3-C4-C5	-9.75	119.97	126.80
33	BA	653	A	N3-C4-C5	-9.75	119.97	126.80
33	BA	829	A	N3-C4-C5	-9.75	119.97	126.80
33	BA	1244	A	N3-C4-C5	-9.75	119.97	126.80
33	BA	1179	A	N3-C4-C5	-9.75	119.97	126.80
33	BA	1453	A	N3-C4-C5	-9.75	119.97	126.80
33	BA	1942	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	117	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	456	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	616	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	644	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	674	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	1257	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	1266	A	N3-C4-C5	-9.75	119.97	126.80
33	BA	247	A	N3-C4-C5	-9.75	119.97	126.80
33	BA	421	A	N3-C4-C5	-9.75	119.97	126.80
33	BA	740	A	N3-C4-C5	-9.75	119.98	126.80
33	BA	1131	A	N3-C4-C5	-9.75	119.97	126.80
34	BB	43	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	519	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	638	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	724	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	1188	A	N3-C4-C5	-9.75	119.98	126.80
33	BA	618	A	N3-C4-C5	-9.75	119.98	126.80
33	BA	781	A	N3-C4-C5	-9.75	119.98	126.80
33	BA	786	A	N3-C4-C5	-9.75	119.98	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1221	A	N3-C4-C5	-9.75	119.98	126.80
33	BA	2875	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	1451	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	67	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	947	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	322	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	993	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	1116	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	1499	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	799	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	1802	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	2007	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	2851	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	160	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1479	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	763	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	204	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	611	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1528	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	176	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	553	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	1654	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	1679	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	2594	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	357	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	618	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	924	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	1466	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	71	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	325	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	1115	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	1913	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	2134	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	2295	A	N3-C4-C5	-9.74	119.98	126.80
33	BA	2191	A	N3-C4-C5	-9.74	119.98	126.80
1	AA	118	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	581	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	1142	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	1314	A	N3-C4-C5	-9.73	119.99	126.80
34	BB	39	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	266	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	816	A	N3-C4-C5	-9.73	119.99	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	125	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	1072	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	1906	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	333	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	544	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	1056	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	1036	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	1465	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	2032	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	258	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	1017	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	342	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	1224	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	62	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	582	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	1161	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	1456	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	1540	A	N3-C4-C5	-9.73	119.99	126.80
33	BA	2417	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	1294	A	N3-C4-C5	-9.72	119.99	126.80
33	BA	1601	A	N3-C4-C5	-9.72	119.99	126.80
33	BA	139	A	N3-C4-C5	-9.72	119.99	126.80
33	BA	161	A	N3-C4-C5	-9.72	119.99	126.80
1	AA	352	A	N3-C4-C5	-9.72	119.99	126.80
1	AA	910	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	969	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	1066	A	N3-C4-C5	-9.72	119.99	126.80
33	BA	198	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	324	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	782	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	1734	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	2480	A	N3-C4-C5	-9.72	120.00	126.80
34	BB	55	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	2364	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	1743	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	704	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	791	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	1261	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	219	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	345	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	677	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	1553	A	N3-C4-C5	-9.72	120.00	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1606	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	2296	A	N3-C4-C5	-9.72	120.00	126.80
33	BA	2297	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	53	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	1296	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	825	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1510	A	N3-C4-C5	-9.71	120.00	126.80
33	BA	1202	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	474	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	757	A	N3-C4-C5	-9.71	120.00	126.80
33	BA	150	A	N3-C4-C5	-9.71	120.00	126.80
33	BA	1957	A	N3-C4-C5	-9.71	120.00	126.80
33	BA	2673	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	929	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1488	A	N3-C4-C5	-9.71	120.00	126.80
33	BA	274	A	N3-C4-C5	-9.71	120.00	126.80
33	BA	1084	A	N3-C4-C5	-9.71	120.00	126.80
33	BA	1326	A	N3-C4-C5	-9.71	120.00	126.80
33	BA	1850	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1225	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1417	A	N3-C4-C5	-9.71	120.01	126.80
33	BA	229	A	N3-C4-C5	-9.71	120.01	126.80
33	BA	659	A	N3-C4-C5	-9.71	120.01	126.80
33	BA	1967	A	N3-C4-C5	-9.71	120.01	126.80
33	BA	2526	A	N3-C4-C5	-9.71	120.01	126.80
1	AA	296	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	541	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	1333	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	1443	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	2132	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	1119	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	1533	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	142	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	210	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	532	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	738	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	302	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	1266	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	476	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	1021	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	1042	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	31	A	N3-C4-C5	-9.70	120.01	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1541	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	1699	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	107	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	202	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	208	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	683	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	2876	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	1818	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	1287	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	2860	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	2923	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	690	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	776	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	823	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	1210	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	1791	A	N3-C4-C5	-9.70	120.01	126.80
34	BB	44	A	N3-C4-C5	-9.70	120.01	126.80
33	BA	2507	A	N3-C4-C5	-9.69	120.01	126.80
33	BA	2767	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	646	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	667	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	463	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	448	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	1504	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	501	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	1205	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	211	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	422	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	1248	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	1386	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	1419	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	1020	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	831	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	154	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	1335	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	1648	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	2482	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	2708	A	N3-C4-C5	-9.69	120.02	126.80
34	BB	102	A	N3-C4-C5	-9.69	120.02	126.80
33	BA	1141	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	329	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	684	A	N3-C4-C5	-9.68	120.02	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	28	A	N3-C4-C5	-9.68	120.02	126.80
33	BA	49	A	N3-C4-C5	-9.68	120.02	126.80
33	BA	582	A	N3-C4-C5	-9.68	120.02	126.80
33	BA	1815	A	N3-C4-C5	-9.68	120.02	126.80
33	BA	2330	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	500	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	1176	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	1197	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	1470	A	N3-C4-C5	-9.68	120.02	126.80
33	BA	1809	A	N3-C4-C5	-9.68	120.02	126.80
34	BB	113	A	N3-C4-C5	-9.68	120.02	126.80
33	BA	179	A	N3-C4-C5	-9.68	120.02	126.80
33	BA	2071	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	228	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	321	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	367	A	N3-C4-C5	-9.68	120.03	126.80
1	AA	651	A	N3-C4-C5	-9.68	120.03	126.80
33	BA	389	A	N3-C4-C5	-9.68	120.03	126.80
33	BA	525	A	N3-C4-C5	-9.68	120.03	126.80
33	BA	727	A	N3-C4-C5	-9.68	120.03	126.80
33	BA	917	A	N3-C4-C5	-9.68	120.03	126.80
33	BA	1014	A	N3-C4-C5	-9.68	120.03	126.80
33	BA	2479	A	N3-C4-C5	-9.68	120.03	126.80
33	BA	1308	A	N3-C4-C5	-9.68	120.03	126.80
33	BA	1722	A	N3-C4-C5	-9.68	120.03	126.80
33	BA	828	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	10	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	120	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	777	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	178	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	206	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	290	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	199	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	273	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	584	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	1092	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	2362	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	2398	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	2912	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	148	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	236	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	460	A	N3-C4-C5	-9.67	120.03	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1503	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	210	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	904	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	2542	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	2908	A	N3-C4-C5	-9.67	120.03	126.80
34	BB	17	A	N3-C4-C5	-9.67	120.03	126.80
34	BB	25	A	N3-C4-C5	-9.67	120.03	126.80
34	BB	37	A	N3-C4-C5	-9.67	120.03	126.80
33	BA	477	A	N3-C4-C5	-9.66	120.03	126.80
33	BA	991	A	N3-C4-C5	-9.66	120.03	126.80
33	BA	1291	A	N3-C4-C5	-9.66	120.03	126.80
1	AA	306	A	N3-C4-C5	-9.66	120.04	126.80
33	BA	224	A	N3-C4-C5	-9.66	120.04	126.80
33	BA	746	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	837	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	159	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	542	A	N3-C4-C5	-9.66	120.04	126.80
33	BA	1175	A	N3-C4-C5	-9.66	120.04	126.80
33	BA	1339	A	N3-C4-C5	-9.66	120.04	126.80
33	BA	2390	A	N3-C4-C5	-9.66	120.04	126.80
33	BA	2770	A	N3-C4-C5	-9.66	120.04	126.80
33	BA	2835	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	775	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	1133	A	N3-C4-C5	-9.66	120.04	126.80
33	BA	202	A	N3-C4-C5	-9.66	120.04	126.80
33	BA	2340	A	N3-C4-C5	-9.66	120.04	126.80
33	BA	2088	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	203	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	1254	A	N3-C4-C5	-9.65	120.04	126.80
33	BA	1914	A	N3-C4-C5	-9.65	120.05	126.80
1	AA	323	A	N3-C4-C5	-9.65	120.05	126.80
1	AA	1050	A	N3-C4-C5	-9.65	120.05	126.80
1	AA	1434	A	N3-C4-C5	-9.65	120.05	126.80
33	BA	314	A	N3-C4-C5	-9.65	120.05	126.80
33	BA	1034	A	N3-C4-C5	-9.65	120.05	126.80
1	AA	1048	A	N3-C4-C5	-9.64	120.05	126.80
33	BA	84	A	N3-C4-C5	-9.64	120.05	126.80
33	BA	1966	A	N3-C4-C5	-9.64	120.05	126.80
33	BA	355	A	N3-C4-C5	-9.64	120.05	126.80
33	BA	475	A	N3-C4-C5	-9.64	120.05	126.80
33	BA	1325	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	189	A	N3-C4-C5	-9.64	120.05	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	925	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	1102	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	1328	A	N3-C4-C5	-9.64	120.05	126.80
33	BA	619	A	N3-C4-C5	-9.64	120.05	126.80
33	BA	702	A	N3-C4-C5	-9.64	120.05	126.80
33	BA	821	A	N3-C4-C5	-9.64	120.05	126.80
33	BA	1189	A	N3-C4-C5	-9.64	120.05	126.80
33	BA	572	A	N3-C4-C5	-9.63	120.06	126.80
33	BA	1929	A	N3-C4-C5	-9.63	120.06	126.80
33	BA	2810	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	386	A	N3-C4-C5	-9.63	120.06	126.80
33	BA	2315	A	N3-C4-C5	-9.63	120.06	126.80
33	BA	1905	A	N3-C4-C5	-9.63	120.06	126.80
33	BA	2059	A	N3-C4-C5	-9.63	120.06	126.80
33	BA	2155	A	N3-C4-C5	-9.63	120.06	126.80
33	BA	166	A	N3-C4-C5	-9.63	120.06	126.80
33	BA	999	A	N3-C4-C5	-9.62	120.06	126.80
33	BA	1434	A	N3-C4-C5	-9.62	120.06	126.80
33	BA	2383	A	N3-C4-C5	-9.62	120.06	126.80
33	BA	2595	A	N3-C4-C5	-9.63	120.06	126.80
33	BA	2804	A	N3-C4-C5	-9.62	120.06	126.80
1	AA	1358	A	N3-C4-C5	-9.62	120.06	126.80
33	BA	1078	A	N3-C4-C5	-9.62	120.06	126.80
1	AA	568	A	N3-C4-C5	-9.62	120.07	126.80
33	BA	717	A	N3-C4-C5	-9.62	120.07	126.80
33	BA	1412	A	N3-C4-C5	-9.62	120.07	126.80
33	BA	1812	A	N3-C4-C5	-9.62	120.07	126.80
33	BA	2375	A	N3-C4-C5	-9.62	120.07	126.80
1	AA	974	A	N3-C4-C5	-9.62	120.07	126.80
33	BA	1149	A	N3-C4-C5	-9.61	120.07	126.80
33	BA	1713	A	N3-C4-C5	-9.61	120.07	126.80
1	AA	438	A	N3-C4-C5	-9.61	120.07	126.80
1	AA	457	A	N3-C4-C5	-9.61	120.08	126.80
1	AA	1289	A	N3-C4-C5	-9.61	120.08	126.80
33	BA	2455	A	N3-C4-C5	-9.61	120.08	126.80
33	BA	244	A	N3-C4-C5	-9.60	120.08	126.80
33	BA	835	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	1207	A	N3-C4-C5	-9.60	120.08	126.80
33	BA	1517	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	583	A	N3-C4-C5	-9.60	120.08	126.80
33	BA	774	A	N3-C4-C5	-9.60	120.08	126.80
33	BA	1123	A	N3-C4-C5	-9.60	120.08	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1579	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	28	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	171	A	N3-C4-C5	-9.59	120.09	126.80
1	AA	730	A	N3-C4-C5	-9.59	120.09	126.80
33	BA	67	A	N3-C4-C5	-9.59	120.09	126.80
33	BA	811	A	N3-C4-C5	-9.59	120.09	126.80
33	BA	1948	A	N3-C4-C5	-9.59	120.09	126.80
33	BA	1347	A	N3-C4-C5	-9.58	120.09	126.80
33	BA	1941	A	N3-C4-C5	-9.58	120.09	126.80
1	AA	975	A	N3-C4-C5	-9.58	120.10	126.80
1	AA	401	A	N3-C4-C5	-9.57	120.10	126.80
33	BA	162	A	N3-C4-C5	-9.57	120.10	126.80
1	AA	569	A	N3-C4-C5	-9.57	120.10	126.80
33	BA	2683	A	N3-C4-C5	-9.57	120.10	126.80
1	AA	713	A	N3-C4-C5	-9.57	120.10	126.80
1	AA	1090	A	N3-C4-C5	-9.57	120.10	126.80
1	AA	151	A	N3-C4-C5	-9.56	120.11	126.80
1	AA	1006	A	N3-C4-C5	-9.56	120.11	126.80
33	BA	1134	A	N7-C8-N9	-9.56	109.02	113.80
33	BA	723	A	N3-C4-C5	-9.56	120.11	126.80
33	BA	2777	A	N3-C4-C5	-9.56	120.11	126.80
1	AA	923	A	N3-C4-C5	-9.55	120.11	126.80
33	BA	1061	A	N3-C4-C5	-9.55	120.11	126.80
33	BA	2276	A	N3-C4-C5	-9.55	120.11	126.80
1	AA	556	A	N3-C4-C5	-9.55	120.12	126.80
1	AA	150	A	N3-C4-C5	-9.55	120.12	126.80
33	BA	1784	A	N3-C4-C5	-9.55	120.12	126.80
33	BA	2254	A	N3-C4-C5	-9.55	120.12	126.80
1	AA	232	A	N3-C4-C5	-9.55	120.12	126.80
33	BA	64	A	N3-C4-C5	-9.55	120.12	126.80
33	BA	1340	A	N3-C4-C5	-9.54	120.12	126.80
33	BA	207	A	N3-C4-C5	-9.53	120.13	126.80
33	BA	2819	A	N3-C4-C5	-9.54	120.12	126.80
1	AA	419	A	N3-C4-C5	-9.53	120.13	126.80
1	AA	1512	A	N3-C4-C5	-9.53	120.13	126.80
33	BA	2262	A	N3-C4-C5	-9.52	120.14	126.80
33	BA	2807	A	N3-C4-C5	-9.52	120.14	126.80
33	BA	575	A	N3-C4-C5	-9.51	120.14	126.80
33	BA	118	A	N3-C4-C5	-9.51	120.14	126.80
33	BA	354	A	N3-C4-C5	-9.51	120.14	126.80
1	AA	18	A	N3-C4-C5	-9.50	120.15	126.80
33	BA	504	A	N3-C4-C5	-9.50	120.15	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	703	A	N3-C4-C5	-9.49	120.15	126.80
33	BA	1844	A	N3-C4-C5	-9.49	120.16	126.80
33	BA	2898	A	N3-C4-C5	-9.49	120.16	126.80
33	BA	1432	A	N3-C4-C5	-9.49	120.16	126.80
33	BA	2618	A	N3-C4-C5	-9.48	120.17	126.80
33	BA	1473	A	N3-C4-C5	-9.48	120.17	126.80
1	AA	1077	A	N3-C4-C5	-9.47	120.17	126.80
33	BA	847	A	N3-C4-C5	-9.47	120.17	126.80
1	AA	254	A	N3-C4-C5	-9.47	120.17	126.80
1	AA	985	A	N3-C4-C5	-9.47	120.17	126.80
33	BA	494	A	N3-C4-C5	-9.46	120.17	126.80
33	BA	1417	A	N3-C4-C5	-9.46	120.18	126.80
33	BA	2606	A	N3-C4-C5	-9.46	120.18	126.80
1	AA	1422	A	N3-C4-C5	-9.46	120.18	126.80
33	BA	490	A	N3-C4-C5	-9.45	120.19	126.80
33	BA	2601	A	N3-C4-C5	-9.45	120.19	126.80
33	BA	126	A	N3-C4-C5	-9.44	120.19	126.80
33	BA	2241	A	N3-C4-C5	-9.44	120.19	126.80
1	AA	209	A	N3-C4-C5	-9.43	120.20	126.80
33	BA	1302	A	N3-C4-C5	-9.43	120.20	126.80
33	BA	2187	A	N3-C4-C5	-9.43	120.20	126.80
33	BA	1919	A	N3-C4-C5	-9.43	120.20	126.80
1	AA	1407	A	N3-C4-C5	-9.42	120.20	126.80
33	BA	1814	A	N3-C4-C5	-9.42	120.20	126.80
33	BA	2670	A	N3-C4-C5	-9.42	120.20	126.80
33	BA	2793	A	N3-C4-C5	-9.42	120.20	126.80
1	AA	899	A	N3-C4-C5	-9.41	120.21	126.80
33	BA	2089	A	N3-C4-C5	-9.41	120.21	126.80
1	AA	1247	A	N3-C4-C5	-9.40	120.22	126.80
1	AA	415	A	N3-C4-C5	-9.40	120.22	126.80
33	BA	526	A	N3-C4-C5	-9.40	120.22	126.80
1	AA	631	A	N3-C4-C5	-9.39	120.23	126.80
1	AA	879	A	N3-C4-C5	-9.39	120.22	126.80
33	BA	1555	A	N3-C4-C5	-9.39	120.23	126.80
33	BA	1188	A	N3-C4-C5	-9.37	120.24	126.80
1	AA	988	A	N3-C4-C5	-9.35	120.26	126.80
1	AA	1355	A	N3-C4-C5	-9.34	120.26	126.80
33	BA	2062	A	N3-C4-C5	-9.34	120.26	126.80
33	BA	647	A	N3-C4-C5	-9.33	120.27	126.80
33	BA	1201	A	N3-C4-C5	-9.33	120.27	126.80
33	BA	1003	A	N3-C4-C5	-9.32	120.27	126.80
33	BA	374	A	N3-C4-C5	-9.31	120.28	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1067	A	N3-C4-C5	-9.30	120.29	126.80
33	BA	1982	A	N3-C4-C5	-9.29	120.30	126.80
33	BA	2916	A	N3-C4-C5	-9.29	120.30	126.80
33	BA	2487	U	C4'-C3'-O3'	9.23	131.47	113.00
33	BA	1305	A	N3-C4-C5	-9.23	120.34	126.80
1	AA	862	A	N3-C4-C5	-9.22	120.34	126.80
33	BA	82	G	C4'-C3'-O3'	-9.21	90.05	109.40
33	BA	501	A	N3-C4-C5	-9.19	120.37	126.80
33	BA	183	A	N3-C4-C5	-9.11	120.42	126.80
1	AA	1372	A	N3-C4-C5	-9.03	120.48	126.80
33	BA	501	A	C5-N7-C8	8.91	108.35	103.90
1	AA	508	A	N3-C4-C5	-8.72	120.69	126.80
33	BA	2805	A	C5-N7-C8	8.66	108.23	103.90
33	BA	527	A	C5-N7-C8	8.61	108.21	103.90
33	BA	722	A	C5-N7-C8	8.57	108.19	103.90
1	AA	1065	A	C5-N7-C8	8.56	108.18	103.90
33	BA	551	A	C5-N7-C8	8.56	108.18	103.90
33	BA	1461	A	C5-N7-C8	8.55	108.17	103.90
1	AA	57	A	C5-N7-C8	8.54	108.17	103.90
33	BA	1895	A	C5-N7-C8	8.52	108.16	103.90
33	BA	2447	A	C5-N7-C8	8.49	108.14	103.90
33	BA	281	A	C5-N7-C8	8.48	108.14	103.90
33	BA	2417	A	C5-N7-C8	8.48	108.14	103.90
1	AA	1133	A	C5-N7-C8	8.48	108.14	103.90
1	AA	10	A	C5-N7-C8	8.47	108.14	103.90
33	BA	1094	A	C5-N7-C8	8.47	108.14	103.90
33	BA	2241	A	C5-N7-C8	8.47	108.14	103.90
33	BA	2049	A	C5-N7-C8	8.47	108.14	103.90
33	BA	1084	A	C5-N7-C8	8.45	108.13	103.90
33	BA	2134	A	C5-N7-C8	8.45	108.12	103.90
1	AA	768	A	C5-N7-C8	8.45	108.12	103.90
1	AA	790	A	C5-N7-C8	8.43	108.11	103.90
33	BA	935	A	C5-N7-C8	8.42	108.11	103.90
1	AA	506	A	C5-N7-C8	8.41	108.11	103.90
33	BA	518	A	C5-N7-C8	8.41	108.11	103.90
1	AA	266	A	C5-N7-C8	8.41	108.11	103.90
33	BA	2364	A	C5-N7-C8	8.41	108.11	103.90
1	AA	886	A	C5-N7-C8	8.41	108.11	103.90
1	AA	1213	A	C5-N7-C8	8.41	108.11	103.90
1	AA	988	A	C5-N7-C8	8.41	108.10	103.90
33	BA	1302	A	C5-N7-C8	8.41	108.10	103.90
33	BA	2782	A	C5-N7-C8	8.41	108.10	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	959	A	C5-N7-C8	8.40	108.10	103.90
1	AA	1320	A	C5-N7-C8	8.40	108.10	103.90
33	BA	538	A	C5-N7-C8	8.40	108.10	103.90
33	BA	690	A	C5-N7-C8	8.40	108.10	103.90
33	BA	1047	A	C5-N7-C8	8.40	108.10	103.90
33	BA	1686	A	C5-N7-C8	8.39	108.10	103.90
1	AA	870	A	C5-N7-C8	8.39	108.10	103.90
33	BA	2026	A	C5-N7-C8	8.38	108.09	103.90
33	BA	2152	A	C5-N7-C8	8.38	108.09	103.90
33	BA	1555	A	C5-N7-C8	8.38	108.09	103.90
33	BA	2464	A	C5-N7-C8	8.38	108.09	103.90
33	BA	2302	A	C5-N7-C8	8.37	108.09	103.90
33	BA	52	A	C5-N7-C8	8.37	108.08	103.90
1	AA	1488	A	C5-N7-C8	8.37	108.08	103.90
1	AA	397	A	C5-N7-C8	8.37	108.08	103.90
33	BA	154	A	C5-N7-C8	8.37	108.08	103.90
33	BA	1189	A	C5-N7-C8	8.37	108.08	103.90
33	BA	1254	A	C5-N7-C8	8.37	108.08	103.90
33	BA	2907	A	C5-N7-C8	8.36	108.08	103.90
33	BA	2750	A	C5-N7-C8	8.36	108.08	103.90
33	BA	1161	A	C5-N7-C8	8.36	108.08	103.90
33	BA	1347	A	C5-N7-C8	8.36	108.08	103.90
33	BA	957	A	C5-N7-C8	8.36	108.08	103.90
33	BA	618	A	C5-N7-C8	8.35	108.08	103.90
33	BA	2315	A	C5-N7-C8	8.35	108.08	103.90
33	BA	2694	A	C5-N7-C8	8.35	108.07	103.90
33	BA	353	A	C5-N7-C8	8.35	108.07	103.90
1	AA	440	A	C5-N7-C8	8.35	108.07	103.90
1	AA	452	A	C5-N7-C8	8.35	108.07	103.90
33	BA	2670	A	C5-N7-C8	8.35	108.07	103.90
1	AA	456	A	C5-N7-C8	8.34	108.07	103.90
33	BA	1809	A	C5-N7-C8	8.34	108.07	103.90
33	BA	2846	A	C5-N7-C8	8.34	108.07	103.90
1	AA	522	A	C5-N7-C8	8.34	108.07	103.90
1	AA	500	A	C5-N7-C8	8.34	108.07	103.90
1	AA	556	A	C5-N7-C8	8.34	108.07	103.90
33	BA	1061	A	C5-N7-C8	8.34	108.07	103.90
33	BA	1524	A	C5-N7-C8	8.33	108.07	103.90
1	AA	737	A	C5-N7-C8	8.33	108.06	103.90
33	BA	1735	A	C5-N7-C8	8.33	108.06	103.90
33	BA	166	A	C5-N7-C8	8.33	108.06	103.90
1	AA	658	A	C5-N7-C8	8.32	108.06	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	752	A	C5-N7-C8	8.32	108.06	103.90
33	BA	888	A	C5-N7-C8	8.32	108.06	103.90
33	BA	1326	A	C5-N7-C8	8.32	108.06	103.90
1	AA	919	A	C5-N7-C8	8.32	108.06	103.90
1	AA	1178	A	C5-N7-C8	8.32	108.06	103.90
33	BA	866	A	C5-N7-C8	8.32	108.06	103.90
33	BA	2594	A	C5-N7-C8	8.32	108.06	103.90
33	BA	526	A	C5-N7-C8	8.32	108.06	103.90
33	BA	2262	A	C5-N7-C8	8.31	108.06	103.90
33	BA	459	A	C5-N7-C8	8.31	108.06	103.90
33	BA	1174	A	C5-N7-C8	8.31	108.06	103.90
34	BB	17	A	C5-N7-C8	8.31	108.06	103.90
1	AA	422	A	C5-N7-C8	8.31	108.05	103.90
33	BA	1585	A	C5-N7-C8	8.31	108.05	103.90
33	BA	2176	A	C5-N7-C8	8.31	108.05	103.90
34	BB	97	A	C5-N7-C8	8.31	108.05	103.90
1	AA	496	A	C5-N7-C8	8.30	108.05	103.90
1	AA	1004	A	C5-N7-C8	8.31	108.05	103.90
33	BA	835	A	C5-N7-C8	8.31	108.05	103.90
33	BA	2163	A	C5-N7-C8	8.31	108.05	103.90
33	BA	2307	A	C5-N7-C8	8.30	108.05	103.90
1	AA	1225	A	C5-N7-C8	8.30	108.05	103.90
33	BA	140	A	C5-N7-C8	8.30	108.05	103.90
33	BA	1483	A	C5-N7-C8	8.30	108.05	103.90
33	BA	2170	A	C5-N7-C8	8.30	108.05	103.90
1	AA	1222	A	C5-N7-C8	8.30	108.05	103.90
1	AA	703	A	C5-N7-C8	8.30	108.05	103.90
33	BA	1202	A	C5-N7-C8	8.30	108.05	103.90
1	AA	232	A	C5-N7-C8	8.30	108.05	103.90
1	AA	1513	A	C5-N7-C8	8.30	108.05	103.90
33	BA	513	A	C4-C5-C6	8.30	121.15	117.00
33	BA	702	A	C5-N7-C8	8.30	108.05	103.90
33	BA	1815	A	C5-N7-C8	8.30	108.05	103.90
1	AA	803	A	C5-N7-C8	8.29	108.05	103.90
1	AA	824	A	C5-N7-C8	8.30	108.05	103.90
33	BA	2807	A	C5-N7-C8	8.29	108.05	103.90
33	BA	2837	A	C5-N7-C8	8.29	108.05	103.90
1	AA	1160	A	C5-N7-C8	8.29	108.05	103.90
33	BA	763	A	C5-N7-C8	8.29	108.05	103.90
33	BA	1115	A	C5-N7-C8	8.29	108.05	103.90
33	BA	2216	A	C5-N7-C8	8.29	108.05	103.90
33	BA	2618	A	C5-N7-C8	8.29	108.05	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1314	A	C5-N7-C8	8.29	108.05	103.90
1	AA	148	A	C5-N7-C8	8.29	108.04	103.90
33	BA	325	A	C5-N7-C8	8.29	108.04	103.90
33	BA	1134	A	N3-C4-N9	8.29	134.03	127.40
33	BA	2923	A	C5-N7-C8	8.29	108.04	103.90
1	AA	811	A	C5-N7-C8	8.29	108.04	103.90
1	AA	796	A	C5-N7-C8	8.28	108.04	103.90
1	AA	1333	A	C5-N7-C8	8.29	108.04	103.90
33	BA	110	A	C5-N7-C8	8.28	108.04	103.90
1	AA	159	A	C5-N7-C8	8.28	108.04	103.90
1	AA	364	A	C5-N7-C8	8.28	108.04	103.90
1	AA	956	A	C5-N7-C8	8.28	108.04	103.90
33	BA	278	A	C5-N7-C8	8.28	108.04	103.90
33	BA	1224	A	C5-N7-C8	8.28	108.04	103.90
33	BA	549	A	C5-N7-C8	8.28	108.04	103.90
33	BA	2462	A	C5-N7-C8	8.28	108.04	103.90
1	AA	862	A	C5-N7-C8	8.28	108.04	103.90
1	AA	1541	A	C5-N7-C8	8.28	108.04	103.90
21	AX	41	A	C5-N7-C8	8.28	108.04	103.90
33	BA	770	A	C5-N7-C8	8.28	108.04	103.90
33	BA	2673	A	C5-N7-C8	8.28	108.04	103.90
33	BA	2902	A	C5-N7-C8	8.28	108.04	103.90
1	AA	206	A	C5-N7-C8	8.28	108.04	103.90
1	AA	189	A	C5-N7-C8	8.28	108.04	103.90
1	AA	475	A	C5-N7-C8	8.28	108.04	103.90
33	BA	302	A	C5-N7-C8	8.28	108.04	103.90
33	BA	1998	A	C5-N7-C8	8.28	108.04	103.90
33	BA	2043	A	C5-N7-C8	8.28	108.04	103.90
33	BA	2398	A	C5-N7-C8	8.28	108.04	103.90
1	AA	203	A	C5-N7-C8	8.27	108.04	103.90
1	AA	251	A	C5-N7-C8	8.27	108.04	103.90
33	BA	991	A	C5-N7-C8	8.27	108.04	103.90
1	AA	367	A	C5-N7-C8	8.27	108.04	103.90
1	AA	786	A	C5-N7-C8	8.27	108.04	103.90
1	AA	690	A	C5-N7-C8	8.27	108.04	103.90
1	AA	254	A	C5-N7-C8	8.27	108.03	103.90
1	AA	1383	A	C5-N7-C8	8.27	108.03	103.90
33	BA	530	A	C5-N7-C8	8.27	108.03	103.90
33	BA	1025	A	C5-N7-C8	8.27	108.03	103.90
1	AA	1510	A	C5-N7-C8	8.27	108.03	103.90
33	BA	322	A	C5-N7-C8	8.27	108.03	103.90
1	AA	704	A	C5-N7-C8	8.27	108.03	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	193	A	C5-N7-C8	8.27	108.03	103.90
33	BA	194	A	C5-N7-C8	8.27	108.03	103.90
33	BA	229	A	C5-N7-C8	8.27	108.03	103.90
33	BA	847	A	C5-N7-C8	8.27	108.03	103.90
33	BA	1190	A	C5-N7-C8	8.27	108.03	103.90
33	BA	1797	A	C5-N7-C8	8.27	108.03	103.90
1	AA	202	A	C5-N7-C8	8.26	108.03	103.90
1	AA	357	A	C5-N7-C8	8.26	108.03	103.90
33	BA	376	A	C5-N7-C8	8.26	108.03	103.90
33	BA	500	A	C5-N7-C8	8.26	108.03	103.90
34	BB	39	A	C5-N7-C8	8.26	108.03	103.90
1	AA	321	A	C5-N7-C8	8.26	108.03	103.90
1	AA	1349	A	C5-N7-C8	8.26	108.03	103.90
33	BA	876	A	C5-N7-C8	8.26	108.03	103.90
33	BA	1243	A	C5-N7-C8	8.26	108.03	103.90
33	BA	1325	A	C5-N7-C8	8.26	108.03	103.90
34	BB	114	A	C5-N7-C8	8.26	108.03	103.90
1	AA	31	A	C5-N7-C8	8.26	108.03	103.90
1	AA	53	A	C5-N7-C8	8.26	108.03	103.90
1	AA	1434	A	C5-N7-C8	8.26	108.03	103.90
33	BA	1078	A	C5-N7-C8	8.26	108.03	103.90
34	BB	43	A	C5-N7-C8	8.26	108.03	103.90
33	BA	582	A	C5-N7-C8	8.25	108.03	103.90
1	AA	178	A	C5-N7-C8	8.25	108.03	103.90
1	AA	204	A	C5-N7-C8	8.25	108.03	103.90
33	BA	1287	A	C5-N7-C8	8.25	108.03	103.90
1	AA	816	A	C5-N7-C8	8.25	108.03	103.90
33	BA	1210	A	C5-N7-C8	8.25	108.03	103.90
33	BA	2777	A	C5-N7-C8	8.25	108.03	103.90
33	BA	2819	A	C5-N7-C8	8.25	108.03	103.90
34	BB	18	A	C5-N7-C8	8.25	108.03	103.90
1	AA	282	A	C5-N7-C8	8.25	108.03	103.90
1	AA	1466	A	C5-N7-C8	8.25	108.03	103.90
33	BA	2317	A	C5-N7-C8	8.25	108.03	103.90
33	BA	2390	A	C5-N7-C8	8.25	108.03	103.90
33	BA	2893	A	C5-N7-C8	8.25	108.03	103.90
33	BA	2683	A	C5-N7-C8	8.25	108.03	103.90
34	BB	27	A	C5-N7-C8	8.25	108.03	103.90
1	AA	419	A	C5-N7-C8	8.25	108.02	103.90
1	AA	1442	A	C5-N7-C8	8.25	108.02	103.90
1	AA	228	A	C5-N7-C8	8.25	108.02	103.90
33	BA	71	A	C5-N7-C8	8.25	108.02	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	125	A	C5-N7-C8	8.25	108.02	103.90
1	AA	170	A	C5-N7-C8	8.24	108.02	103.90
1	AA	329	A	C5-N7-C8	8.24	108.02	103.90
1	AA	460	A	C5-N7-C8	8.24	108.02	103.90
1	AA	501	A	C5-N7-C8	8.24	108.02	103.90
1	AA	532	A	C5-N7-C8	8.24	108.02	103.90
1	AA	672	A	C5-N7-C8	8.24	108.02	103.90
33	BA	275	A	C5-N7-C8	8.24	108.02	103.90
33	BA	476	A	C5-N7-C8	8.24	108.02	103.90
33	BA	1654	A	C5-N7-C8	8.24	108.02	103.90
33	BA	2700	A	C5-N7-C8	8.24	108.02	103.90
33	BA	2722	A	C5-N7-C8	8.24	108.02	103.90
1	AA	918	A	C5-N7-C8	8.24	108.02	103.90
33	BA	389	A	C5-N7-C8	8.24	108.02	103.90
33	BA	1286	A	C5-N7-C8	8.24	108.02	103.90
33	BA	1784	A	C5-N7-C8	8.24	108.02	103.90
33	BA	1966	A	C5-N7-C8	8.24	108.02	103.90
33	BA	2119	A	C5-N7-C8	8.24	108.02	103.90
33	BA	2132	A	C5-N7-C8	8.24	108.02	103.90
33	BA	2155	A	C5-N7-C8	8.24	108.02	103.90
1	AA	1284	A	C5-N7-C8	8.24	108.02	103.90
33	BA	2330	A	C5-N7-C8	8.24	108.02	103.90
1	AA	1384	A	C5-N7-C8	8.24	108.02	103.90
33	BA	407	A	C5-N7-C8	8.24	108.02	103.90
1	AA	139	A	C5-N7-C8	8.23	108.02	103.90
1	AA	281	A	C5-N7-C8	8.23	108.02	103.90
33	BA	2668	A	C5-N7-C8	8.23	108.02	103.90
33	BA	1464	A	C5-N7-C8	8.23	108.02	103.90
1	AA	1348	A	C5-N7-C8	8.23	108.02	103.90
1	AA	1509	A	C5-N7-C8	8.23	108.02	103.90
33	BA	1592	A	C5-N7-C8	8.23	108.02	103.90
1	AA	582	A	C5-N7-C8	8.23	108.02	103.90
33	BA	307	A	C5-N7-C8	8.23	108.02	103.90
33	BA	449	A	C5-N7-C8	8.23	108.02	103.90
33	BA	1504	A	C5-N7-C8	8.23	108.02	103.90
33	BA	1553	A	C5-N7-C8	8.23	108.02	103.90
33	BA	2100	A	C5-N7-C8	8.23	108.02	103.90
33	BA	150	A	C5-N7-C8	8.23	108.01	103.90
33	BA	1335	A	C5-N7-C8	8.23	108.02	103.90
33	BA	1392	A	C5-N7-C8	8.23	108.01	103.90
33	BA	2854	A	C5-N7-C8	8.23	108.01	103.90
33	BA	236	A	C5-N7-C8	8.23	108.01	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	412	A	C5-N7-C8	8.23	108.01	103.90
33	BA	717	A	C5-N7-C8	8.23	108.01	103.90
33	BA	922	A	C5-N7-C8	8.23	108.01	103.90
33	BA	1913	A	C5-N7-C8	8.23	108.01	103.90
33	BA	2089	A	C5-N7-C8	8.23	108.01	103.90
33	BA	2298	A	C5-N7-C8	8.23	108.01	103.90
1	AA	947	A	C5-N7-C8	8.22	108.01	103.90
1	AA	1112	A	C5-N7-C8	8.22	108.01	103.90
1	AA	1266	A	C5-N7-C8	8.22	108.01	103.90
33	BA	646	A	C5-N7-C8	8.22	108.01	103.90
33	BA	1277	A	C5-N7-C8	8.22	108.01	103.90
33	BA	1588	A	C5-N7-C8	8.22	108.01	103.90
33	BA	2191	A	C5-N7-C8	8.22	108.01	103.90
33	BA	2338	A	C5-N7-C8	8.22	108.01	103.90
33	BA	2770	A	C5-N7-C8	8.22	108.01	103.90
33	BA	2071	A	C5-N7-C8	8.22	108.01	103.90
33	BA	2329	A	C5-N7-C8	8.22	108.01	103.90
1	AA	917	A	C5-N7-C8	8.22	108.01	103.90
33	BA	364	A	C5-N7-C8	8.22	108.01	103.90
33	BA	1034	A	C5-N7-C8	8.22	108.01	103.90
1	AA	1443	A	C5-N7-C8	8.22	108.01	103.90
1	AA	1493	A	C5-N7-C8	8.22	108.01	103.90
1	AA	1503	A	C5-N7-C8	8.22	108.01	103.90
33	BA	2351	A	C5-N7-C8	8.22	108.01	103.90
1	AA	928	A	C5-N7-C8	8.22	108.01	103.90
33	BA	519	A	C5-N7-C8	8.22	108.01	103.90
33	BA	829	A	C5-N7-C8	8.22	108.01	103.90
33	BA	1631	A	C5-N7-C8	8.22	108.01	103.90
33	BA	2052	A	C5-N7-C8	8.22	108.01	103.90
1	AA	664	A	C5-N7-C8	8.22	108.01	103.90
1	AA	791	A	C5-N7-C8	8.21	108.01	103.90
1	AA	1257	A	C5-N7-C8	8.21	108.01	103.90
33	BA	421	A	C5-N7-C8	8.21	108.01	103.90
33	BA	637	A	C5-N7-C8	8.21	108.01	103.90
33	BA	821	A	C5-N7-C8	8.21	108.01	103.90
33	BA	1008	A	C5-N7-C8	8.21	108.01	103.90
33	BA	1059	A	C5-N7-C8	8.21	108.01	103.90
33	BA	1619	A	C5-N7-C8	8.21	108.01	103.90
33	BA	1942	A	C5-N7-C8	8.21	108.01	103.90
1	AA	333	A	C5-N7-C8	8.21	108.01	103.90
1	AA	923	A	C5-N7-C8	8.21	108.01	103.90
21	AX	14	A	C5-N7-C8	8.21	108.01	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2500	A	C5-N7-C8	8.21	108.01	103.90
1	AA	1147	A	C5-N7-C8	8.21	108.01	103.90
1	AA	1248	A	C5-N7-C8	8.21	108.00	103.90
33	BA	947	A	C5-N7-C8	8.21	108.00	103.90
1	AA	611	A	C5-N7-C8	8.21	108.00	103.90
1	AA	828	A	C5-N7-C8	8.21	108.00	103.90
33	BA	429	A	C5-N7-C8	8.21	108.00	103.90
33	BA	507	A	C5-N7-C8	8.21	108.00	103.90
33	BA	999	A	C5-N7-C8	8.21	108.00	103.90
33	BA	1144	A	C5-N7-C8	8.21	108.00	103.90
33	BA	2362	A	C5-N7-C8	8.21	108.00	103.90
33	BA	2606	A	C5-N7-C8	8.21	108.00	103.90
33	BA	2769	A	C5-N7-C8	8.21	108.00	103.90
33	BA	2830	A	C5-N7-C8	8.21	108.00	103.90
1	AA	287	A	C5-N7-C8	8.21	108.00	103.90
33	BA	572	A	C5-N7-C8	8.21	108.00	103.90
33	BA	1260	A	C5-N7-C8	8.21	108.00	103.90
1	AA	1456	A	C5-N7-C8	8.20	108.00	103.90
33	BA	765	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1534	A	C5-N7-C8	8.21	108.00	103.90
33	BA	1699	A	C5-N7-C8	8.21	108.00	103.90
1	AA	240	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1523	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1528	A	C5-N7-C8	8.20	108.00	103.90
33	BA	130	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1490	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1961	A	C5-N7-C8	8.20	108.00	103.90
1	AA	651	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1205	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1269	A	C5-N7-C8	8.20	108.00	103.90
33	BA	2812	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1254	A	C5-N7-C8	8.20	108.00	103.90
33	BA	14	A	C5-N7-C8	8.20	108.00	103.90
33	BA	553	A	C5-N7-C8	8.20	108.00	103.90
33	BA	575	A	C5-N7-C8	8.20	108.00	103.90
33	BA	578	A	C5-N7-C8	8.20	108.00	103.90
33	BA	868	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1029	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1233	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1679	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1260	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1341	A	C5-N7-C8	8.20	108.00	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	161	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1055	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1175	A	C5-N7-C8	8.20	108.00	103.90
33	BA	600	A	C5-N7-C8	8.20	108.00	103.90
33	BA	667	A	C5-N7-C8	8.19	108.00	103.90
33	BA	1179	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1393	A	C5-N7-C8	8.20	108.00	103.90
33	BA	1700	A	C5-N7-C8	8.19	108.00	103.90
1	AA	94	A	C5-N7-C8	8.19	108.00	103.90
1	AA	477	A	C5-N7-C8	8.19	108.00	103.90
1	AA	899	A	C5-N7-C8	8.19	108.00	103.90
1	AA	1185	A	C5-N7-C8	8.19	108.00	103.90
1	AA	1419	A	C5-N7-C8	8.19	108.00	103.90
33	BA	1046	A	C5-N7-C8	8.19	108.00	103.90
33	BA	2088	A	C5-N7-C8	8.19	108.00	103.90
1	AA	1502	A	C5-N7-C8	8.19	108.00	103.90
33	BA	44	A	C5-N7-C8	8.19	108.00	103.90
33	BA	677	A	C5-N7-C8	8.19	108.00	103.90
33	BA	952	A	C5-N7-C8	8.19	108.00	103.90
33	BA	1073	A	C5-N7-C8	8.19	108.00	103.90
33	BA	1339	A	C5-N7-C8	8.19	108.00	103.90
33	BA	1745	A	C5-N7-C8	8.19	108.00	103.90
33	BA	1802	A	C5-N7-C8	8.19	108.00	103.90
1	AA	529	A	C5-N7-C8	8.19	108.00	103.90
1	AA	638	A	C5-N7-C8	8.19	108.00	103.90
1	AA	669	A	C5-N7-C8	8.19	108.00	103.90
1	AA	671	A	C5-N7-C8	8.19	108.00	103.90
1	AA	1102	A	C5-N7-C8	8.19	108.00	103.90
33	BA	5	A	C5-N7-C8	8.19	108.00	103.90
33	BA	1813	A	C5-N7-C8	8.19	108.00	103.90
1	AA	1252	A	C5-N7-C8	8.19	107.99	103.90
33	BA	179	A	C5-N7-C8	8.19	107.99	103.90
33	BA	925	A	C5-N7-C8	8.19	108.00	103.90
33	BA	1230	A	C5-N7-C8	8.19	107.99	103.90
33	BA	1636	A	C5-N7-C8	8.19	107.99	103.90
33	BA	2106	A	C5-N7-C8	8.19	107.99	103.90
33	BA	715	A	C5-N7-C8	8.19	107.99	103.90
33	BA	1235	A	C5-N7-C8	8.19	107.99	103.90
1	AA	62	A	C5-N7-C8	8.19	107.99	103.90
1	AA	1028	A	C5-N7-C8	8.19	107.99	103.90
1	AA	1103	A	C5-N7-C8	8.19	107.99	103.90
1	AA	1121	A	C5-N7-C8	8.19	107.99	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	543	A	C5-N7-C8	8.19	107.99	103.90
33	BA	870	A	C5-N7-C8	8.19	107.99	103.90
33	BA	893	A	C5-N7-C8	8.19	107.99	103.90
33	BA	1375	A	C5-N7-C8	8.19	107.99	103.90
33	BA	1685	A	C5-N7-C8	8.19	107.99	103.90
33	BA	2904	A	C5-N7-C8	8.19	107.99	103.90
1	AA	401	A	C5-N7-C8	8.18	107.99	103.90
33	BA	2165	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1050	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1271	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1386	A	C5-N7-C8	8.18	107.99	103.90
33	BA	108	A	C5-N7-C8	8.18	107.99	103.90
33	BA	279	A	C5-N7-C8	8.18	107.99	103.90
33	BA	388	A	C5-N7-C8	8.18	107.99	103.90
33	BA	428	A	C5-N7-C8	8.18	107.99	103.90
33	BA	2276	A	C5-N7-C8	8.18	107.99	103.90
33	BA	2511	A	C5-N7-C8	8.18	107.99	103.90
33	BA	2889	A	C5-N7-C8	8.18	107.99	103.90
1	AA	978	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1259	A	C5-N7-C8	8.18	107.99	103.90
33	BA	345	A	C5-N7-C8	8.18	107.99	103.90
33	BA	1313	A	C5-N7-C8	8.18	107.99	103.90
1	AA	234	A	C5-N7-C8	8.18	107.99	103.90
1	AA	512	A	C5-N7-C8	8.18	107.99	103.90
33	BA	369	A	C5-N7-C8	8.18	107.99	103.90
33	BA	1005	A	C5-N7-C8	8.18	107.99	103.90
1	AA	581	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1077	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1529	A	C5-N7-C8	8.18	107.99	103.90
33	BA	173	A	C5-N7-C8	8.18	107.99	103.90
33	BA	1423	A	C5-N7-C8	8.18	107.99	103.90
33	BA	1653	A	C5-N7-C8	8.18	107.99	103.90
33	BA	2787	A	C5-N7-C8	8.18	107.99	103.90
33	BA	2835	A	C5-N7-C8	8.18	107.99	103.90
33	BA	2876	A	C5-N7-C8	8.18	107.99	103.90
1	AA	225	A	C5-N7-C8	8.18	107.99	103.90
1	AA	925	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1197	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1234	A	C5-N7-C8	8.18	107.99	103.90
21	AX	44	A	C5-N7-C8	8.18	107.99	103.90
33	BA	1312	A	C5-N7-C8	8.18	107.99	103.90
1	AA	190	A	C5-N7-C8	8.17	107.99	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	544	A	C5-N7-C8	8.17	107.99	103.90
1	AA	1451	A	C5-N7-C8	8.17	107.99	103.90
21	AX	21	A	C5-N7-C8	8.17	107.99	103.90
33	BA	965	A	C5-N7-C8	8.17	107.99	103.90
33	BA	1072	A	C5-N7-C8	8.17	107.99	103.90
33	BA	1096	A	C5-N7-C8	8.17	107.99	103.90
33	BA	1617	A	C5-N7-C8	8.17	107.99	103.90
33	BA	2658	A	C5-N7-C8	8.17	107.99	103.90
1	AA	12	A	C5-N7-C8	8.17	107.98	103.90
1	AA	715	A	C5-N7-C8	8.17	107.98	103.90
1	AA	721	A	C5-N7-C8	8.17	107.98	103.90
1	AA	771	A	C5-N7-C8	8.17	107.98	103.90
33	BA	987	A	C5-N7-C8	8.17	107.98	103.90
33	BA	652	A	C5-N7-C8	8.17	107.98	103.90
33	BA	758	A	C5-N7-C8	8.17	107.98	103.90
33	BA	1516	A	C5-N7-C8	8.17	107.99	103.90
33	BA	1014	A	C5-N7-C8	8.17	107.98	103.90
33	BA	1838	A	C5-N7-C8	8.17	107.98	103.90
34	BB	76	A	C5-N7-C8	8.17	107.98	103.90
1	AA	382	A	C5-N7-C8	8.17	107.98	103.90
1	AA	423	A	C5-N7-C8	8.17	107.98	103.90
33	BA	49	A	C5-N7-C8	8.17	107.98	103.90
33	BA	2860	A	C5-N7-C8	8.17	107.98	103.90
1	AA	616	A	C5-N7-C8	8.17	107.98	103.90
1	AA	757	A	C5-N7-C8	8.17	107.98	103.90
1	AA	985	A	C5-N7-C8	8.17	107.98	103.90
1	AA	1425	A	C5-N7-C8	8.17	107.98	103.90
33	BA	2297	A	C5-N7-C8	8.17	107.98	103.90
33	BA	185	A	C5-N7-C8	8.17	107.98	103.90
33	BA	1473	A	C5-N7-C8	8.17	107.98	103.90
33	BA	1778	A	C5-N7-C8	8.17	107.98	103.90
33	BA	2047	A	C5-N7-C8	8.17	107.98	103.90
33	BA	2383	A	C5-N7-C8	8.17	107.98	103.90
1	AA	1092	A	C5-N7-C8	8.16	107.98	103.90
1	AA	361	A	C5-N7-C8	8.16	107.98	103.90
1	AA	568	A	C5-N7-C8	8.16	107.98	103.90
1	AA	569	A	C5-N7-C8	8.16	107.98	103.90
1	AA	777	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1437	A	C5-N7-C8	8.16	107.98	103.90
33	BA	517	A	C5-N7-C8	8.16	107.98	103.90
33	BA	705	A	C5-N7-C8	8.16	107.98	103.90
33	BA	740	A	C5-N7-C8	8.16	107.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1157	A	C5-N7-C8	8.16	107.98	103.90
33	BA	1967	A	C5-N7-C8	8.16	107.98	103.90
34	BB	44	A	C5-N7-C8	8.16	107.98	103.90
1	AA	725	A	C5-N7-C8	8.16	107.98	103.90
33	BA	67	A	C5-N7-C8	8.16	107.98	103.90
33	BA	1608	A	C5-N7-C8	8.16	107.98	103.90
33	BA	1982	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1427	A	C5-N7-C8	8.16	107.98	103.90
33	BA	260	A	C5-N7-C8	8.16	107.98	103.90
33	BA	584	A	C5-N7-C8	8.16	107.98	103.90
33	BA	1346	A	C5-N7-C8	8.16	107.98	103.90
1	AA	76	A	C5-N7-C8	8.16	107.98	103.90
1	AA	236	A	C5-N7-C8	8.16	107.98	103.90
1	AA	799	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1298	A	C5-N7-C8	8.16	107.98	103.90
33	BA	782	A	C5-N7-C8	8.16	107.98	103.90
33	BA	1583	A	C5-N7-C8	8.16	107.98	103.90
33	BA	1831	A	C5-N7-C8	8.16	107.98	103.90
33	BA	2018	A	C5-N7-C8	8.16	107.98	103.90
1	AA	160	A	C5-N7-C8	8.16	107.98	103.90
1	AA	371	A	C5-N7-C8	8.16	107.98	103.90
1	AA	433	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1054	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1210	A	C5-N7-C8	8.16	107.98	103.90
33	BA	10	A	C5-N7-C8	8.16	107.98	103.90
33	BA	12	A	C5-N7-C8	8.16	107.98	103.90
33	BA	219	A	C5-N7-C8	8.16	107.98	103.90
33	BA	220	A	C5-N7-C8	8.16	107.98	103.90
33	BA	274	A	C5-N7-C8	8.16	107.98	103.90
33	BA	769	A	C5-N7-C8	8.16	107.98	103.90
33	BA	1142	A	C5-N7-C8	8.16	107.98	103.90
33	BA	418	A	C5-N7-C8	8.16	107.98	103.90
33	BA	882	A	C5-N7-C8	8.16	107.98	103.90
33	BA	1308	A	C5-N7-C8	8.16	107.98	103.90
33	BA	1540	A	C5-N7-C8	8.16	107.98	103.90
33	BA	1405	A	C5-N7-C8	8.16	107.98	103.90
33	BA	2227	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1111	A	C5-N7-C8	8.15	107.98	103.90
1	AA	1176	A	C5-N7-C8	8.15	107.98	103.90
33	BA	231	A	C5-N7-C8	8.15	107.98	103.90
1	AA	389	A	C5-N7-C8	8.15	107.98	103.90
1	AA	1115	A	C5-N7-C8	8.15	107.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2220	A	C5-N7-C8	8.15	107.98	103.90
1	AA	1120	A	C5-N7-C8	8.15	107.98	103.90
1	AA	1417	A	C5-N7-C8	8.15	107.98	103.90
33	BA	13	A	C5-N7-C8	8.15	107.98	103.90
33	BA	504	A	C5-N7-C8	8.15	107.98	103.90
33	BA	117	A	C5-N7-C8	8.15	107.98	103.90
33	BA	244	A	C5-N7-C8	8.15	107.98	103.90
33	BA	337	A	C5-N7-C8	8.15	107.98	103.90
33	BA	653	A	C5-N7-C8	8.15	107.98	103.90
33	BA	1677	A	C5-N7-C8	8.15	107.98	103.90
33	BA	2062	A	C5-N7-C8	8.15	107.98	103.90
33	BA	2827	A	C5-N7-C8	8.15	107.98	103.90
1	AA	404	A	C5-N7-C8	8.15	107.97	103.90
1	AA	462	A	C5-N7-C8	8.15	107.98	103.90
1	AA	541	A	C5-N7-C8	8.15	107.98	103.90
1	AA	762	A	C5-N7-C8	8.15	107.98	103.90
1	AA	910	A	C5-N7-C8	8.15	107.98	103.90
1	AA	945	A	C5-N7-C8	8.15	107.98	103.90
1	AA	1355	A	C5-N7-C8	8.15	107.98	103.90
1	AA	1486	A	C5-N7-C8	8.15	107.97	103.90
33	BA	324	A	C5-N7-C8	8.15	107.98	103.90
33	BA	436	A	C5-N7-C8	8.15	107.98	103.90
33	BA	917	A	C5-N7-C8	8.15	107.98	103.90
33	BA	2256	A	C5-N7-C8	8.15	107.98	103.90
33	BA	2601	A	C5-N7-C8	8.15	107.98	103.90
33	BA	2912	A	C5-N7-C8	8.15	107.98	103.90
33	BA	171	A	C5-N7-C8	8.15	107.97	103.90
33	BA	1141	A	C5-N7-C8	8.15	107.97	103.90
33	BA	1445	A	C5-N7-C8	8.15	107.97	103.90
1	AA	61	A	C5-N7-C8	8.15	107.97	103.90
1	AA	405	A	C5-N7-C8	8.15	107.97	103.90
33	BA	786	A	C5-N7-C8	8.15	107.97	103.90
33	BA	2034	A	C5-N7-C8	8.15	107.97	103.90
1	AA	18	A	C5-N7-C8	8.15	107.97	103.90
1	AA	211	A	C5-N7-C8	8.15	107.97	103.90
1	AA	258	A	C5-N7-C8	8.15	107.97	103.90
1	AA	696	A	C5-N7-C8	8.15	107.97	103.90
33	BA	547	A	C5-N7-C8	8.15	107.97	103.90
33	BA	1593	A	C5-N7-C8	8.15	107.97	103.90
33	BA	1945	A	C5-N7-C8	8.15	107.97	103.90
1	AA	55	A	C5-N7-C8	8.14	107.97	103.90
1	AA	107	A	C5-N7-C8	8.14	107.97	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1369	A	C5-N7-C8	8.14	107.97	103.90
1	AA	118	A	C5-N7-C8	8.14	107.97	103.90
1	AA	210	A	C5-N7-C8	8.14	107.97	103.90
1	AA	335	A	C5-N7-C8	8.14	107.97	103.90
1	AA	776	A	C5-N7-C8	8.14	107.97	103.90
1	AA	1179	A	C5-N7-C8	8.14	107.97	103.90
33	BA	978	A	C5-N7-C8	8.14	107.97	103.90
1	AA	1490	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2356	A	C5-N7-C8	8.14	107.97	103.90
33	BA	479	A	C5-N7-C8	8.14	107.97	103.90
33	BA	1357	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2027	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2148	A	C5-N7-C8	8.14	107.97	103.90
1	AA	659	A	C5-N7-C8	8.14	107.97	103.90
33	BA	225	A	C5-N7-C8	8.14	107.97	103.90
33	BA	1710	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2369	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2463	A	C5-N7-C8	8.14	107.97	103.90
33	BA	207	A	C5-N7-C8	8.14	107.97	103.90
33	BA	314	A	C5-N7-C8	8.14	107.97	103.90
1	AA	1403	A	C5-N7-C8	8.14	107.97	103.90
21	AX	58	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2007	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2087	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2455	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2542	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2740	A	C5-N7-C8	8.14	107.97	103.90
33	BA	183	A	C5-N7-C8	8.14	107.97	103.90
1	AA	801	A	C5-N7-C8	8.13	107.97	103.90
1	AA	1188	A	C5-N7-C8	8.13	107.97	103.90
1	AA	1327	A	C5-N7-C8	8.13	107.97	103.90
1	AA	1435	A	C5-N7-C8	8.13	107.97	103.90
33	BA	224	A	C5-N7-C8	8.13	107.97	103.90
33	BA	456	A	C5-N7-C8	8.14	107.97	103.90
33	BA	867	A	C5-N7-C8	8.13	107.97	103.90
33	BA	1021	A	C5-N7-C8	8.13	107.97	103.90
33	BA	1424	A	C5-N7-C8	8.14	107.97	103.90
33	BA	1845	A	C5-N7-C8	8.14	107.97	103.90
33	BA	2826	A	C5-N7-C8	8.14	107.97	103.90
33	BA	1925	A	C5-N7-C8	8.13	107.97	103.90
33	BA	2316	A	C5-N7-C8	8.13	107.97	103.90
33	BA	2629	A	C5-N7-C8	8.13	107.97	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2762	A	C5-N7-C8	8.13	107.97	103.90
33	BA	2845	A	C5-N7-C8	8.13	107.97	103.90
1	AA	386	A	C5-N7-C8	8.13	107.97	103.90
33	BA	333	A	C5-N7-C8	8.13	107.97	103.90
1	AA	271	A	C5-N7-C8	8.13	107.97	103.90
1	AA	618	A	C5-N7-C8	8.13	107.97	103.90
33	BA	974	A	C5-N7-C8	8.13	107.97	103.90
33	BA	2406	A	C5-N7-C8	8.13	107.97	103.90
33	BA	2477	A	C5-N7-C8	8.13	107.97	103.90
1	AA	337	A	C5-N7-C8	8.13	107.97	103.90
1	AA	879	A	C5-N7-C8	8.13	107.97	103.90
1	AA	924	A	C5-N7-C8	8.13	107.97	103.90
33	BA	178	A	C5-N7-C8	8.13	107.97	103.90
33	BA	619	A	C5-N7-C8	8.13	107.97	103.90
33	BA	889	A	C5-N7-C8	8.13	107.97	103.90
33	BA	1947	A	C5-N7-C8	8.13	107.97	103.90
33	BA	2146	A	C5-N7-C8	8.13	107.97	103.90
33	BA	2421	A	C5-N7-C8	8.13	107.97	103.90
33	BA	2810	A	C5-N7-C8	8.13	107.97	103.90
33	BA	2834	A	C5-N7-C8	8.13	107.97	103.90
34	BB	51	A	C5-N7-C8	8.13	107.97	103.90
1	AA	1359	A	C5-N7-C8	8.13	107.97	103.90
33	BA	64	A	C5-N7-C8	8.13	107.97	103.90
33	BA	330	A	C5-N7-C8	8.13	107.97	103.90
33	BA	1406	A	C5-N7-C8	8.13	107.97	103.90
1	AA	649	A	C5-N7-C8	8.13	107.96	103.90
1	AA	738	A	C5-N7-C8	8.13	107.96	103.90
21	AX	70	A	C5-N7-C8	8.13	107.96	103.90
33	BA	808	A	C5-N7-C8	8.13	107.96	103.90
33	BA	1092	A	C5-N7-C8	8.13	107.96	103.90
33	BA	1663	A	C5-N7-C8	8.13	107.96	103.90
33	BA	1722	A	C5-N7-C8	8.13	107.97	103.90
33	BA	1948	A	C5-N7-C8	8.13	107.96	103.90
33	BA	2059	A	C5-N7-C8	8.13	107.96	103.90
1	AA	679	A	C5-N7-C8	8.12	107.96	103.90
33	BA	2507	A	C5-N7-C8	8.13	107.96	103.90
1	AA	1422	A	C5-N7-C8	8.12	107.96	103.90
33	BA	258	A	C5-N7-C8	8.12	107.96	103.90
33	BA	762	A	C5-N7-C8	8.12	107.96	103.90
33	BA	828	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1194	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1648	A	C5-N7-C8	8.12	107.96	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1791	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1901	A	C5-N7-C8	8.12	107.96	103.90
33	BA	305	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1812	A	C5-N7-C8	8.12	107.96	103.90
1	AA	129	A	C5-N7-C8	8.12	107.96	103.90
33	BA	94	A	C5-N7-C8	8.12	107.96	103.90
33	BA	273	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1020	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1734	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1918	A	C5-N7-C8	8.12	107.96	103.90
33	BA	2395	A	C5-N7-C8	8.12	107.96	103.90
33	BA	2459	A	C5-N7-C8	8.12	107.96	103.90
1	AA	208	A	C5-N7-C8	8.12	107.96	103.90
33	BA	318	A	C5-N7-C8	8.12	107.96	103.90
33	BA	753	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1026	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1323	A	C5-N7-C8	8.12	107.96	103.90
34	BB	56	A	C5-N7-C8	8.12	107.96	103.90
1	AA	604	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1128	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1207	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1580	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1426	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1569	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1776	A	C5-N7-C8	8.12	107.96	103.90
33	BA	2327	A	C5-N7-C8	8.12	107.96	103.90
33	BA	2900	A	C5-N7-C8	8.12	107.96	103.90
34	BB	102	A	C5-N7-C8	8.12	107.96	103.90
1	AA	1328	A	C5-N7-C8	8.12	107.96	103.90
33	BA	124	A	C5-N7-C8	8.12	107.96	103.90
33	BA	2200	A	C5-N7-C8	8.12	107.96	103.90
1	AA	463	A	C5-N7-C8	8.11	107.96	103.90
1	AA	650	A	C5-N7-C8	8.11	107.96	103.90
1	AA	1512	A	C5-N7-C8	8.11	107.96	103.90
33	BA	144	A	C5-N7-C8	8.11	107.96	103.90
33	BA	326	A	C5-N7-C8	8.11	107.96	103.90
33	BA	896	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1027	A	C5-N7-C8	8.11	107.96	103.90
33	BA	1253	A	C5-N7-C8	8.11	107.96	103.90
33	BA	1627	A	C5-N7-C8	8.12	107.96	103.90
33	BA	1638	A	C5-N7-C8	8.11	107.96	103.90
33	BA	2030	A	C5-N7-C8	8.12	107.96	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2187	A	C5-N7-C8	8.12	107.96	103.90
33	BA	2560	A	C5-N7-C8	8.12	107.96	103.90
1	AA	195	A	C5-N7-C8	8.11	107.96	103.90
1	AA	685	A	C5-N7-C8	8.11	107.96	103.90
1	AA	711	A	C5-N7-C8	8.11	107.96	103.90
1	AA	974	A	C5-N7-C8	8.11	107.96	103.90
1	AA	1270	A	C5-N7-C8	8.11	107.96	103.90
33	BA	2387	A	C5-N7-C8	8.11	107.96	103.90
1	AA	1048	A	C5-N7-C8	8.11	107.96	103.90
1	AA	1056	A	C5-N7-C8	8.11	107.96	103.90
1	AA	1479	A	C5-N7-C8	8.11	107.96	103.90
33	BA	28	A	C5-N7-C8	8.11	107.96	103.90
33	BA	548	A	C5-N7-C8	8.11	107.95	103.90
33	BA	1743	A	C5-N7-C8	8.11	107.96	103.90
33	BA	1989	A	C5-N7-C8	8.11	107.96	103.90
1	AA	67	A	C5-N7-C8	8.11	107.95	103.90
1	AA	270	A	C5-N7-C8	8.11	107.95	103.90
1	AA	968	A	C5-N7-C8	8.11	107.95	103.90
33	BA	470	A	C5-N7-C8	8.11	107.95	103.90
33	BA	329	A	C5-N7-C8	8.11	107.95	103.90
33	BA	475	A	C5-N7-C8	8.11	107.95	103.90
33	BA	1888	A	C5-N7-C8	8.11	107.95	103.90
33	BA	2570	A	C5-N7-C8	8.11	107.95	103.90
33	BA	139	A	C5-N7-C8	8.11	107.95	103.90
1	AA	301	A	C5-N7-C8	8.11	107.95	103.90
1	AA	415	A	C5-N7-C8	8.11	107.95	103.90
33	BA	477	A	C5-N7-C8	8.11	107.95	103.90
33	BA	970	A	C5-N7-C8	8.11	107.95	103.90
1	AA	1017	A	C5-N7-C8	8.11	107.95	103.90
33	BA	1709	A	C5-N7-C8	8.11	107.95	103.90
33	BA	1906	A	C5-N7-C8	8.11	107.95	103.90
34	BB	55	A	C5-N7-C8	8.11	107.95	103.90
1	AA	485	A	C5-N7-C8	8.10	107.95	103.90
1	AA	542	A	C5-N7-C8	8.10	107.95	103.90
1	AA	831	A	C5-N7-C8	8.10	107.95	103.90
33	BA	469	A	C5-N7-C8	8.10	107.95	103.90
33	BA	1499	A	C5-N7-C8	8.10	107.95	103.90
33	BA	1575	A	C5-N7-C8	8.10	107.95	103.90
33	BA	2270	A	C5-N7-C8	8.10	107.95	103.90
33	BA	2340	A	C5-N7-C8	8.10	107.95	103.90
33	BA	2661	A	C5-N7-C8	8.10	107.95	103.90
1	AA	793	A	C5-N7-C8	8.10	107.95	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1180	A	C5-N7-C8	8.10	107.95	103.90
33	BA	102	A	C5-N7-C8	8.10	107.95	103.90
33	BA	1981	A	C5-N7-C8	8.10	107.95	103.90
33	BA	2042	A	C5-N7-C8	8.10	107.95	103.90
33	BA	2919	A	C5-N7-C8	8.10	107.95	103.90
1	AA	592	A	C5-N7-C8	8.10	107.95	103.90
1	AA	730	A	C5-N7-C8	8.10	107.95	103.90
33	BA	781	A	C5-N7-C8	8.10	107.95	103.90
33	BA	1876	A	C5-N7-C8	8.10	107.95	103.90
34	BB	11	A	C5-N7-C8	8.10	107.95	103.90
33	BA	259	A	C5-N7-C8	8.10	107.95	103.90
33	BA	373	A	C5-N7-C8	8.10	107.95	103.90
33	BA	1956	A	C5-N7-C8	8.10	107.95	103.90
34	BB	105	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1006	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1245	A	C5-N7-C8	8.10	107.95	103.90
33	BA	1417	A	C5-N7-C8	8.10	107.95	103.90
1	AA	296	A	C5-N7-C8	8.09	107.95	103.90
33	BA	384	A	C5-N7-C8	8.09	107.95	103.90
33	BA	622	A	C5-N7-C8	8.09	107.95	103.90
1	AA	677	A	C5-N7-C8	8.09	107.95	103.90
1	AA	1206	A	C5-N7-C8	8.09	107.95	103.90
33	BA	1517	A	C5-N7-C8	8.09	107.95	103.90
33	BA	2869	A	C5-N7-C8	8.09	107.95	103.90
1	AA	72	A	C5-N7-C8	8.09	107.94	103.90
1	AA	128	A	C5-N7-C8	8.09	107.94	103.90
1	AA	1090	A	C5-N7-C8	8.09	107.94	103.90
1	AA	459	A	C5-N7-C8	8.09	107.94	103.90
33	BA	65	A	C5-N7-C8	8.09	107.94	103.90
33	BA	176	A	C5-N7-C8	8.09	107.94	103.90
33	BA	1914	A	C5-N7-C8	8.09	107.95	103.90
33	BA	222	A	C5-N7-C8	8.09	107.94	103.90
33	BA	574	A	C5-N7-C8	8.09	107.94	103.90
33	BA	1839	A	C5-N7-C8	8.09	107.94	103.90
33	BA	2590	A	C5-N7-C8	8.09	107.94	103.90
1	AA	1140	A	C5-N7-C8	8.09	107.94	103.90
1	AA	1455	A	C5-N7-C8	8.09	107.94	103.90
33	BA	216	A	C5-N7-C8	8.09	107.94	103.90
1	AA	35	A	C5-N7-C8	8.09	107.94	103.90
1	AA	52	A	C5-N7-C8	8.09	107.94	103.90
33	BA	683	A	C5-N7-C8	8.09	107.94	103.90
33	BA	73	A	C5-N7-C8	8.09	107.94	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1480	A	C5-N7-C8	8.09	107.94	103.90
33	BA	1618	A	C5-N7-C8	8.09	107.94	103.90
33	BA	1746	A	C5-N7-C8	8.09	107.94	103.90
33	BA	2643	A	C5-N7-C8	8.09	107.94	103.90
33	BA	2851	A	C5-N7-C8	8.09	107.94	103.90
34	BB	25	A	C5-N7-C8	8.09	107.94	103.90
1	AA	142	A	C5-N7-C8	8.08	107.94	103.90
1	AA	1283	A	C5-N7-C8	8.08	107.94	103.90
33	BA	126	A	C5-N7-C8	8.08	107.94	103.90
33	BA	1113	A	C5-N7-C8	8.08	107.94	103.90
33	BA	1818	A	C5-N7-C8	8.08	107.94	103.90
33	BA	1066	A	C5-N7-C8	8.08	107.94	103.90
33	BA	1123	A	C5-N7-C8	8.08	107.94	103.90
33	BA	2381	A	C5-N7-C8	8.08	107.94	103.90
33	BA	2532	A	C5-N7-C8	8.08	107.94	103.90
33	BA	2686	A	C5-N7-C8	8.08	107.94	103.90
1	AA	120	A	C5-N7-C8	8.08	107.94	103.90
1	AA	823	A	C5-N7-C8	8.08	107.94	103.90
1	AA	1200	A	C5-N7-C8	8.08	107.94	103.90
33	BA	1542	A	C5-N7-C8	8.08	107.94	103.90
1	AA	913	A	C5-N7-C8	8.08	107.94	103.90
33	BA	133	A	C5-N7-C8	8.08	107.94	103.90
1	AA	81	A	C5-N7-C8	8.08	107.94	103.90
1	AA	883	A	C5-N7-C8	8.08	107.94	103.90
33	BA	1532	A	C5-N7-C8	8.08	107.94	103.90
33	BA	2663	A	C5-N7-C8	8.08	107.94	103.90
1	AA	308	A	C5-N7-C8	8.07	107.94	103.90
1	AA	314	A	C5-N7-C8	8.07	107.94	103.90
33	BA	38	A	C5-N7-C8	8.07	107.94	103.90
1	AA	1407	A	C5-N7-C8	8.07	107.94	103.90
33	BA	268	A	C5-N7-C8	8.07	107.94	103.90
33	BA	630	A	C5-N7-C8	8.07	107.94	103.90
33	BA	851	A	C5-N7-C8	8.07	107.94	103.90
33	BA	1533	A	C5-N7-C8	8.07	107.94	103.90
33	BA	1562	A	C5-N7-C8	8.07	107.94	103.90
1	AA	140	A	C5-N7-C8	8.07	107.94	103.90
1	AA	838	A	C5-N7-C8	8.07	107.94	103.90
1	AA	844	A	C5-N7-C8	8.07	107.94	103.90
1	AA	902	A	C5-N7-C8	8.07	107.94	103.90
33	BA	1100	A	C5-N7-C8	8.07	107.94	103.90
33	BA	1885	A	C5-N7-C8	8.07	107.94	103.90
33	BA	2295	A	C5-N7-C8	8.07	107.94	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1258	A	C5-N7-C8	8.07	107.93	103.90
33	BA	2000	A	C5-N7-C8	8.07	107.94	103.90
33	BA	2402	A	C5-N7-C8	8.07	107.94	103.90
33	BA	2571	A	C5-N7-C8	8.07	107.94	103.90
33	BA	2794	A	C5-N7-C8	8.07	107.93	103.90
1	AA	1014	A	C5-N7-C8	8.07	107.93	103.90
33	BA	1075	A	C5-N7-C8	8.07	107.93	103.90
1	AA	929	A	C5-N7-C8	8.07	107.93	103.90
33	BA	168	A	C5-N7-C8	8.07	107.93	103.90
33	BA	2804	A	C5-N7-C8	8.07	107.93	103.90
33	BA	692	A	C5-N7-C8	8.07	107.93	103.90
33	BA	746	A	C5-N7-C8	8.07	107.93	103.90
33	BA	993	A	C5-N7-C8	8.07	107.93	103.90
33	BA	1284	A	C5-N7-C8	8.07	107.93	103.90
33	BA	1672	A	C5-N7-C8	8.07	107.93	103.90
33	BA	1723	A	C5-N7-C8	8.07	107.93	103.90
33	BA	2078	A	C5-N7-C8	8.07	107.93	103.90
33	BA	2407	A	C5-N7-C8	8.07	107.93	103.90
33	BA	2547	A	C5-N7-C8	8.07	107.93	103.90
33	BA	2662	A	C5-N7-C8	8.07	107.93	103.90
33	BA	2767	A	C5-N7-C8	8.07	107.93	103.90
33	BA	437	A	C5-N7-C8	8.06	107.93	103.90
33	BA	2111	A	C5-N7-C8	8.06	107.93	103.90
33	BA	2343	A	C5-N7-C8	8.06	107.93	103.90
33	BA	2461	A	C5-N7-C8	8.06	107.93	103.90
33	BA	2482	A	C5-N7-C8	8.06	107.93	103.90
33	BA	2734	A	C5-N7-C8	8.06	107.93	103.90
1	AA	161	A	C5-N7-C8	8.06	107.93	103.90
1	AA	278	A	C5-N7-C8	8.06	107.93	103.90
1	AA	674	A	C5-N7-C8	8.06	107.93	103.90
33	BA	6	A	C5-N7-C8	8.06	107.93	103.90
33	BA	2619	A	C5-N7-C8	8.06	107.93	103.90
33	BA	486	A	C5-N7-C8	8.06	107.93	103.90
33	BA	1789	A	C5-N7-C8	8.06	107.93	103.90
33	BA	2143	A	C5-N7-C8	8.06	107.93	103.90
34	BB	113	A	C5-N7-C8	8.06	107.93	103.90
1	AA	1256	A	C5-N7-C8	8.06	107.93	103.90
33	BA	943	A	C5-N7-C8	8.06	107.93	103.90
33	BA	559	A	C5-N7-C8	8.06	107.93	103.90
33	BA	592	A	C5-N7-C8	8.06	107.93	103.90
34	BB	46	A	C5-N7-C8	8.06	107.93	103.90
1	AA	306	A	C5-N7-C8	8.05	107.93	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	346	A	C5-N7-C8	8.06	107.93	103.90
1	AA	372	A	C5-N7-C8	8.05	107.93	103.90
1	AA	518	A	C5-N7-C8	8.06	107.93	103.90
1	AA	979	A	C5-N7-C8	8.06	107.93	103.90
1	AA	1289	A	C5-N7-C8	8.05	107.93	103.90
1	AA	1296	A	C5-N7-C8	8.06	107.93	103.90
33	BA	206	A	C5-N7-C8	8.05	107.93	103.90
33	BA	342	A	C5-N7-C8	8.05	107.93	103.90
33	BA	1201	A	C5-N7-C8	8.05	107.93	103.90
33	BA	1675	A	C5-N7-C8	8.05	107.93	103.90
33	BA	1929	A	C5-N7-C8	8.05	107.93	103.90
33	BA	1995	A	C5-N7-C8	8.05	107.93	103.90
1	AA	34	A	C5-N7-C8	8.05	107.93	103.90
1	AA	617	A	C5-N7-C8	8.05	107.93	103.90
33	BA	2497	A	C5-N7-C8	8.05	107.93	103.90
1	AA	705	A	C5-N7-C8	8.05	107.92	103.90
1	AA	1026	A	C5-N7-C8	8.05	107.92	103.90
1	AA	1297	A	C5-N7-C8	8.05	107.92	103.90
33	BA	524	A	C5-N7-C8	8.05	107.92	103.90
33	BA	964	A	C5-N7-C8	8.05	107.93	103.90
33	BA	1126	A	C5-N7-C8	8.05	107.93	103.90
33	BA	1957	A	C5-N7-C8	8.05	107.93	103.90
33	BA	2303	A	C5-N7-C8	8.05	107.92	103.90
33	BA	2365	A	C5-N7-C8	8.05	107.92	103.90
33	BA	2831	A	C5-N7-C8	8.05	107.93	103.90
33	BA	1036	A	C5-N7-C8	8.05	107.92	103.90
33	BA	1536	A	C5-N7-C8	8.05	107.92	103.90
33	BA	2389	A	C5-N7-C8	8.05	107.92	103.90
33	BA	2593	A	C5-N7-C8	8.05	107.92	103.90
33	BA	2790	A	C5-N7-C8	8.05	107.92	103.90
1	AA	290	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2124	A	C5-N7-C8	8.05	107.92	103.90
1	AA	352	A	C5-N7-C8	8.04	107.92	103.90
1	AA	390	A	C5-N7-C8	8.04	107.92	103.90
1	AA	1031	A	C5-N7-C8	8.04	107.92	103.90
33	BA	202	A	C5-N7-C8	8.05	107.92	103.90
33	BA	198	A	C5-N7-C8	8.04	107.92	103.90
33	BA	727	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2505	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2526	A	C5-N7-C8	8.04	107.92	103.90
1	AA	605	A	C5-N7-C8	8.04	107.92	103.90
1	AA	644	A	C5-N7-C8	8.04	107.92	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	561	A	C5-N7-C8	8.04	107.92	103.90
33	BA	658	A	C5-N7-C8	8.04	107.92	103.90
33	BA	894	A	C5-N7-C8	8.04	107.92	103.90
33	BA	1116	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2405	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2228	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2436	A	C5-N7-C8	8.04	107.92	103.90
1	AA	117	A	C5-N7-C8	8.04	107.92	103.90
1	AA	1478	A	C5-N7-C8	8.04	107.92	103.90
21	AX	76	A	C5-N7-C8	8.04	107.92	103.90
33	BA	374	A	C5-N7-C8	8.04	107.92	103.90
33	BA	724	A	C5-N7-C8	8.04	107.92	103.90
33	BA	1132	A	C5-N7-C8	8.04	107.92	103.90
33	BA	1421	A	C5-N7-C8	8.04	107.92	103.90
33	BA	1615	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2044	A	C5-N7-C8	8.04	107.92	103.90
1	AA	74	A	C5-N7-C8	8.04	107.92	103.90
33	BA	230	A	C5-N7-C8	8.04	107.92	103.90
33	BA	354	A	C5-N7-C8	8.04	107.92	103.90
33	BA	661	A	C5-N7-C8	8.04	107.92	103.90
33	BA	1149	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2117	A	C5-N7-C8	8.04	107.92	103.90
33	BA	1316	A	C5-N7-C8	8.04	107.92	103.90
33	BA	1882	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2060	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2339	A	C5-N7-C8	8.04	107.92	103.90
33	BA	2908	A	C5-N7-C8	8.04	107.92	103.90
1	AA	630	A	C5-N7-C8	8.04	107.92	103.90
1	AA	1024	A	C5-N7-C8	8.04	107.92	103.90
21	AX	9	A	C5-N7-C8	8.04	107.92	103.90
33	BA	21	A	C5-N7-C8	8.04	107.92	103.90
33	BA	41	A	C5-N7-C8	8.04	107.92	103.90
33	BA	1054	A	C5-N7-C8	8.04	107.92	103.90
33	BA	1456	A	C5-N7-C8	8.04	107.92	103.90
33	BA	1760	A	C5-N7-C8	8.03	107.92	103.90
1	AA	504	A	C5-N7-C8	8.03	107.92	103.90
33	BA	355	A	C5-N7-C8	8.03	107.92	103.90
33	BA	736	A	C5-N7-C8	8.03	107.92	103.90
33	BA	560	A	C5-N7-C8	8.03	107.92	103.90
33	BA	1360	A	C5-N7-C8	8.03	107.92	103.90
33	BA	1788	A	C5-N7-C8	8.03	107.92	103.90
33	BA	1848	A	C5-N7-C8	8.03	107.92	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2006	A	C5-N7-C8	8.03	107.92	103.90
33	BA	2357	A	C5-N7-C8	8.03	107.92	103.90
1	AA	837	A	C5-N7-C8	8.03	107.91	103.90
1	AA	1463	A	C5-N7-C8	8.03	107.91	103.90
33	BA	200	A	C5-N7-C8	8.03	107.91	103.90
33	BA	390	A	C5-N7-C8	8.03	107.91	103.90
33	BA	1197	A	C5-N7-C8	8.03	107.91	103.90
33	BA	1442	A	C5-N7-C8	8.03	107.91	103.90
33	BA	2254	A	C5-N7-C8	8.03	107.91	103.90
33	BA	2440	A	C5-N7-C8	8.03	107.91	103.90
33	BA	2754	A	C5-N7-C8	8.03	107.91	103.90
33	BA	431	A	C5-N7-C8	8.03	107.91	103.90
33	BA	490	A	C5-N7-C8	8.03	107.91	103.90
33	BA	537	A	C5-N7-C8	8.03	107.91	103.90
33	BA	1131	A	C5-N7-C8	8.03	107.91	103.90
34	BB	37	A	C5-N7-C8	8.03	107.91	103.90
33	BA	1003	A	C5-N7-C8	8.03	107.91	103.90
33	BA	2066	A	C5-N7-C8	8.03	107.91	103.90
33	BA	2875	A	C5-N7-C8	8.03	107.91	103.90
1	AA	1143	A	C5-N7-C8	8.02	107.91	103.90
33	BA	2141	A	C5-N7-C8	8.02	107.91	103.90
1	AA	323	A	C5-N7-C8	8.02	107.91	103.90
33	BA	84	A	C5-N7-C8	8.02	107.91	103.90
33	BA	1042	A	C5-N7-C8	8.02	107.91	103.90
21	AX	24	A	C5-N7-C8	8.02	107.91	103.90
33	BA	156	A	C5-N7-C8	8.02	107.91	103.90
33	BA	723	A	C5-N7-C8	8.02	107.91	103.90
33	BA	948	A	C5-N7-C8	8.02	107.91	103.90
33	BA	1266	A	C5-N7-C8	8.02	107.91	103.90
33	BA	1477	A	C5-N7-C8	8.02	107.91	103.90
33	BA	1905	A	C5-N7-C8	8.02	107.91	103.90
33	BA	2375	A	C5-N7-C8	8.02	107.91	103.90
33	BA	811	A	C5-N7-C8	8.02	107.91	103.90
33	BA	1103	A	C5-N7-C8	8.02	107.91	103.90
33	BA	1541	A	C5-N7-C8	8.02	107.91	103.90
33	BA	2779	A	C5-N7-C8	8.02	107.91	103.90
1	AA	28	A	C5-N7-C8	8.02	107.91	103.90
33	BA	1999	A	C5-N7-C8	8.02	107.91	103.90
33	BA	265	A	C5-N7-C8	8.01	107.91	103.90
1	AA	474	A	C5-N7-C8	8.01	107.91	103.90
33	BA	1130	A	C5-N7-C8	8.01	107.91	103.90
33	BA	2205	A	C5-N7-C8	8.01	107.91	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2479	A	C5-N7-C8	8.01	107.91	103.90
33	BA	448	A	C5-N7-C8	8.01	107.91	103.90
1	AA	173	A	C5-N7-C8	8.01	107.91	103.90
1	AA	684	A	C5-N7-C8	8.01	107.91	103.90
33	BA	343	A	C5-N7-C8	8.01	107.90	103.90
33	BA	1388	A	C5-N7-C8	8.01	107.91	103.90
33	BA	1506	A	C5-N7-C8	8.01	107.91	103.90
33	BA	2924	A	C5-N7-C8	8.01	107.91	103.90
34	BB	50	A	C5-N7-C8	8.01	107.91	103.90
1	AA	171	A	C5-N7-C8	8.01	107.90	103.90
33	BA	673	A	C5-N7-C8	8.01	107.90	103.90
1	AA	1405	A	C5-N7-C8	8.01	107.90	103.90
33	BA	1453	A	C5-N7-C8	8.01	107.90	103.90
33	BA	2719	A	C5-N7-C8	8.01	107.90	103.90
1	AA	825	A	C5-N7-C8	8.00	107.90	103.90
33	BA	1119	A	C5-N7-C8	8.00	107.90	103.90
33	BA	1900	A	C5-N7-C8	8.00	107.90	103.90
33	BA	849	A	C5-N7-C8	8.00	107.90	103.90
33	BA	1556	A	C5-N7-C8	8.00	107.90	103.90
33	BA	2517	A	C5-N7-C8	8.00	107.90	103.90
33	BA	2887	A	C5-N7-C8	8.00	107.90	103.90
33	BA	391	A	C5-N7-C8	8.00	107.90	103.90
33	BA	1465	A	C5-N7-C8	8.00	107.90	103.90
1	AA	1022	A	C5-N7-C8	8.00	107.90	103.90
33	BA	1265	A	C5-N7-C8	8.00	107.90	103.90
33	BA	2091	A	C5-N7-C8	8.00	107.90	103.90
1	AA	775	A	C5-N7-C8	8.00	107.90	103.90
1	AA	984	A	C5-N7-C8	8.00	107.90	103.90
33	BA	1074	A	C5-N7-C8	8.00	107.90	103.90
33	BA	2454	A	C5-N7-C8	8.00	107.90	103.90
1	AA	491	A	C5-N7-C8	8.00	107.90	103.90
33	BA	1844	A	C5-N7-C8	8.00	107.90	103.90
33	BA	2498	A	C5-N7-C8	8.00	107.90	103.90
33	BA	1695	A	C5-N7-C8	7.99	107.90	103.90
33	BA	2164	A	C5-N7-C8	7.99	107.90	103.90
33	BA	1941	A	C5-N7-C8	7.99	107.90	103.90
33	BA	2708	A	C5-N7-C8	7.99	107.90	103.90
1	AA	743	A	C5-N7-C8	7.99	107.89	103.90
33	BA	254	A	C5-N7-C8	7.99	107.89	103.90
33	BA	1614	A	C5-N7-C8	7.99	107.89	103.90
1	AA	758	A	C5-N7-C8	7.99	107.89	103.90
1	AA	1247	A	C5-N7-C8	7.99	107.89	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	199	A	C5-N7-C8	7.99	107.89	103.90
33	BA	438	A	C5-N7-C8	7.99	107.89	103.90
33	BA	1222	A	C5-N7-C8	7.99	107.89	103.90
33	BA	2441	A	C5-N7-C8	7.99	107.89	103.90
33	BA	2885	A	C5-N7-C8	7.98	107.89	103.90
33	BA	1434	A	C5-N7-C8	7.98	107.89	103.90
33	BA	1724	A	C5-N7-C8	7.98	107.89	103.90
33	BA	2032	A	C5-N7-C8	7.98	107.89	103.90
34	BB	71	A	C5-N7-C8	7.98	107.89	103.90
33	BA	339	A	C5-N7-C8	7.98	107.89	103.90
34	BB	64	A	C5-N7-C8	7.98	107.89	103.90
1	AA	381	A	C5-N7-C8	7.98	107.89	103.90
1	AA	724	A	C5-N7-C8	7.98	107.89	103.90
1	AA	572	A	C5-N7-C8	7.97	107.89	103.90
33	BA	162	A	C5-N7-C8	7.97	107.89	103.90
33	BA	689	A	C5-N7-C8	7.97	107.89	103.90
33	BA	699	A	C5-N7-C8	7.97	107.89	103.90
33	BA	247	A	C5-N7-C8	7.97	107.89	103.90
33	BA	1727	A	C5-N7-C8	7.97	107.89	103.90
33	BA	1965	A	C5-N7-C8	7.97	107.89	103.90
33	BA	2704	A	C5-N7-C8	7.97	107.89	103.90
33	BA	1221	A	C5-N7-C8	7.97	107.89	103.90
33	BA	1404	A	C5-N7-C8	7.97	107.89	103.90
33	BA	1291	A	C5-N7-C8	7.97	107.88	103.90
33	BA	1697	A	C5-N7-C8	7.97	107.88	103.90
33	BA	1432	A	C5-N7-C8	7.96	107.88	103.90
33	BA	2627	A	C5-N7-C8	7.96	107.88	103.90
1	AA	1261	A	C5-N7-C8	7.96	107.88	103.90
33	BA	1381	A	C5-N7-C8	7.96	107.88	103.90
1	AA	975	A	C5-N7-C8	7.96	107.88	103.90
1	AA	1288	A	C5-N7-C8	7.96	107.88	103.90
1	AA	1315	A	C5-N7-C8	7.96	107.88	103.90
1	AA	987	A	C5-N7-C8	7.96	107.88	103.90
1	AA	1308	A	C5-N7-C8	7.96	107.88	103.90
33	BA	1520	A	C5-N7-C8	7.96	107.88	103.90
33	BA	2844	A	C5-N7-C8	7.96	107.88	103.90
33	BA	623	A	C5-N7-C8	7.96	107.88	103.90
33	BA	910	A	C5-N7-C8	7.96	107.88	103.90
1	AA	1342	A	C5-N7-C8	7.95	107.88	103.90
33	BA	91	A	C5-N7-C8	7.95	107.88	103.90
1	AA	1272	A	C5-N7-C8	7.95	107.88	103.90
33	BA	790	A	C5-N7-C8	7.95	107.87	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1655	A	C5-N7-C8	7.95	107.87	103.90
33	BA	1850	A	C5-N7-C8	7.95	107.87	103.90
1	AA	519	A	C5-N7-C8	7.95	107.87	103.90
1	AA	875	A	C5-N7-C8	7.95	107.87	103.90
1	AA	996	A	C5-N7-C8	7.94	107.87	103.90
33	BA	1361	A	C5-N7-C8	7.94	107.87	103.90
33	BA	525	A	C5-N7-C8	7.94	107.87	103.90
33	BA	956	A	C5-N7-C8	7.94	107.87	103.90
33	BA	659	A	C5-N7-C8	7.94	107.87	103.90
33	BA	61	A	C5-N7-C8	7.94	107.87	103.90
33	BA	616	A	C5-N7-C8	7.93	107.87	103.90
33	BA	1767	A	C5-N7-C8	7.93	107.87	103.90
1	AA	1155	A	C5-N7-C8	7.93	107.87	103.90
1	AA	1236	A	C5-N7-C8	7.93	107.87	103.90
33	BA	593	A	C5-N7-C8	7.93	107.87	103.90
33	BA	971	A	C5-N7-C8	7.93	107.87	103.90
33	BA	1768	A	C5-N7-C8	7.93	107.87	103.90
33	BA	2349	A	C5-N7-C8	7.93	107.87	103.90
1	AA	391	A	C5-N7-C8	7.93	107.86	103.90
33	BA	1601	A	C5-N7-C8	7.93	107.86	103.90
1	AA	583	A	C5-N7-C8	7.93	107.86	103.90
33	BA	1877	A	C5-N7-C8	7.93	107.86	103.90
1	AA	150	A	C5-N7-C8	7.93	107.86	103.90
1	AA	438	A	C5-N7-C8	7.92	107.86	103.90
33	BA	1620	A	C5-N7-C8	7.92	107.86	103.90
33	BA	2252	A	C5-N7-C8	7.92	107.86	103.90
33	BA	958	A	C5-N7-C8	7.92	107.86	103.90
1	AA	1517	A	C5-N7-C8	7.92	107.86	103.90
33	BA	678	A	C5-N7-C8	7.92	107.86	103.90
33	BA	1485	A	C5-N7-C8	7.92	107.86	103.90
1	AA	911	A	C5-N7-C8	7.92	107.86	103.90
33	BA	1680	A	C5-N7-C8	7.92	107.86	103.90
33	BA	1713	A	C5-N7-C8	7.92	107.86	103.90
33	BA	1305	A	C5-N7-C8	7.92	107.86	103.90
1	AA	969	A	C5-N7-C8	7.91	107.85	103.90
33	BA	904	A	C5-N7-C8	7.91	107.85	103.90
33	BA	2080	A	C5-N7-C8	7.91	107.85	103.90
33	BA	2689	A	C5-N7-C8	7.91	107.85	103.90
33	BA	1667	A	C5-N7-C8	7.90	107.85	103.90
1	AA	344	A	C5-N7-C8	7.90	107.85	103.90
1	AA	631	A	C5-N7-C8	7.90	107.85	103.90
33	BA	1412	A	C5-N7-C8	7.90	107.85	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1832	A	C5-N7-C8	7.89	107.85	103.90
33	BA	1858	A	C5-N7-C8	7.89	107.84	103.90
1	AA	1189	A	C5-N7-C8	7.89	107.84	103.90
34	BB	13	A	C5-N7-C8	7.89	107.84	103.90
33	BA	210	A	C5-N7-C8	7.89	107.84	103.90
33	BA	2616	A	C5-N7-C8	7.89	107.84	103.90
1	AA	882	A	C5-N7-C8	7.88	107.84	103.90
33	BA	2595	A	C5-N7-C8	7.88	107.84	103.90
33	BA	908	A	C5-N7-C8	7.88	107.84	103.90
33	BA	1930	A	C5-N7-C8	7.88	107.84	103.90
33	BA	2202	A	C5-N7-C8	7.88	107.84	103.90
1	AA	948	A	C5-N7-C8	7.88	107.84	103.90
33	BA	2848	A	C5-N7-C8	7.88	107.84	103.90
1	AA	151	A	C5-N7-C8	7.87	107.84	103.90
33	BA	2862	A	C5-N7-C8	7.87	107.84	103.90
33	BA	2691	A	C5-N7-C8	7.87	107.83	103.90
33	BA	1019	A	C5-N7-C8	7.87	107.83	103.90
33	BA	1883	A	C5-N7-C8	7.87	107.83	103.90
1	AA	1470	A	C5-N7-C8	7.87	107.83	103.90
33	BA	1721	A	C5-N7-C8	7.87	107.83	103.90
33	BA	1606	A	C5-N7-C8	7.86	107.83	103.90
1	AA	209	A	C5-N7-C8	7.86	107.83	103.90
33	BA	913	A	C5-N7-C8	7.86	107.83	103.90
33	BA	1714	A	C5-N7-C8	7.86	107.83	103.90
1	AA	874	A	C5-N7-C8	7.85	107.83	103.90
34	BB	20	A	C5-N7-C8	7.85	107.83	103.90
33	BA	1691	A	C5-N7-C8	7.85	107.83	103.90
21	AX	23	A	C5-N7-C8	7.85	107.83	103.90
33	BA	1056	A	C5-N7-C8	7.85	107.82	103.90
33	BA	1581	A	C5-N7-C8	7.84	107.82	103.90
1	AA	727	A	C5-N7-C8	7.84	107.82	103.90
1	AA	1238	A	C5-N7-C8	7.84	107.82	103.90
33	BA	830	A	C5-N7-C8	7.84	107.82	103.90
33	BA	462	A	C5-N7-C8	7.84	107.82	103.90
1	AA	1278	A	C5-N7-C8	7.83	107.82	103.90
33	BA	2358	A	C5-N7-C8	7.83	107.82	103.90
33	BA	2898	A	C5-N7-C8	7.83	107.82	103.90
33	BA	774	A	C5-N7-C8	7.83	107.81	103.90
33	BA	2735	A	C5-N7-C8	7.83	107.82	103.90
33	BA	1579	A	C5-N7-C8	7.83	107.81	103.90
1	AA	1294	A	C5-N7-C8	7.83	107.81	103.90
1	AA	555	A	C5-N7-C8	7.83	107.81	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2296	A	C5-N7-C8	7.83	107.81	103.90
33	BA	2480	A	C5-N7-C8	7.82	107.81	103.90
33	BA	2793	A	C5-N7-C8	7.82	107.81	103.90
33	BA	647	A	C5-N7-C8	7.81	107.81	103.90
33	BA	2778	A	C5-N7-C8	7.81	107.81	103.90
33	BA	1820	A	C5-N7-C8	7.81	107.80	103.90
33	BA	2123	A	C5-N7-C8	7.81	107.80	103.90
33	BA	1097	A	C5-N7-C8	7.80	107.80	103.90
33	BA	226	A	C5-N7-C8	7.79	107.80	103.90
1	AA	1166	A	C5-N7-C8	7.79	107.80	103.90
33	BA	656	A	C5-N7-C8	7.78	107.79	103.90
33	BA	1006	A	C5-N7-C8	7.78	107.79	103.90
1	AA	1161	A	C5-N7-C8	7.78	107.79	103.90
1	AA	114	A	C5-N7-C8	7.77	107.79	103.90
1	AA	548	A	C5-N7-C8	7.77	107.79	103.90
33	BA	1816	A	C5-N7-C8	7.77	107.79	103.90
33	BA	2083	A	C5-N7-C8	7.77	107.78	103.90
1	AA	1016	A	C5-N7-C8	7.76	107.78	103.90
1	AA	993	A	C5-N7-C8	7.75	107.77	103.90
1	AA	508	A	C5-N7-C8	7.73	107.77	103.90
33	BA	90	A	C5-N7-C8	7.73	107.76	103.90
33	BA	1244	A	C5-N7-C8	7.73	107.76	103.90
33	BA	1491	A	C5-N7-C8	7.73	107.76	103.90
1	AA	1026	A	C4-C5-C6	7.72	120.86	117.00
33	BA	95	A	C5-N7-C8	7.72	107.76	103.90
33	BA	496	A	C5-N7-C8	7.72	107.76	103.90
33	BA	1173	A	C5'-C4'-O4'	7.72	118.36	109.10
33	BA	56	A	C5-N7-C8	7.71	107.75	103.90
33	BA	53	A	C5-N7-C8	7.71	107.75	103.90
1	AA	1366	A	C5-N7-C8	7.70	107.75	103.90
33	BA	2916	A	C5-N7-C8	7.70	107.75	103.90
33	BA	1814	A	C5-N7-C8	7.69	107.74	103.90
33	BA	2468	A	C5-N7-C8	7.68	107.74	103.90
1	AA	713	A	C5-N7-C8	7.68	107.74	103.90
33	BA	2786	A	C5-N7-C8	7.67	107.73	103.90
33	BA	513	A	C5-N7-C8	7.67	107.73	103.90
33	BA	1928	A	C5-N7-C8	7.66	107.73	103.90
1	AA	99	A	C5-N7-C8	7.66	107.73	103.90
1	AA	457	A	C5-N7-C8	7.66	107.73	103.90
1	AA	1372	A	C5-N7-C8	7.63	107.72	103.90
33	BA	679	A	C5-N7-C8	7.63	107.72	103.90
1	AA	933	A	C5-N7-C8	7.63	107.71	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1358	A	C5-N7-C8	7.62	107.71	103.90
33	BA	634	A	C5-N7-C8	7.61	107.71	103.90
33	BA	226	A	N3-C4-N9	7.60	133.48	127.40
33	BA	1134	A	C4-C5-C6	7.60	120.80	117.00
1	AA	1308	A	N3-C4-N9	7.58	133.47	127.40
33	BA	1340	A	C5-N7-C8	7.58	107.69	103.90
33	BA	1691	A	N3-C4-N9	7.58	133.46	127.40
33	BA	118	A	C5-N7-C8	7.57	107.68	103.90
33	BA	1919	A	C5-N7-C8	7.56	107.68	103.90
33	BA	1134	A	C5-N7-C8	7.55	107.67	103.90
33	BA	1774	A	C5-N7-C8	7.55	107.67	103.90
33	BA	1398	A	C5-N7-C8	7.55	107.67	103.90
33	BA	1714	A	N3-C4-N9	7.55	133.44	127.40
1	AA	405	A	N3-C4-N9	7.54	133.43	127.40
33	BA	366	A	C4'-C3'-O3'	7.52	128.03	113.00
33	BA	2627	A	C4-C5-C6	7.51	120.75	117.00
1	AA	507	A	C5-N7-C8	7.49	107.65	103.90
33	BA	494	A	C5-N7-C8	7.49	107.64	103.90
33	BA	1006	A	C4-C5-C6	7.47	120.74	117.00
33	BA	2885	A	C4-C5-C6	7.45	120.72	117.00
34	BB	99	A	C4-C5-C6	7.41	120.70	117.00
33	BA	478	U	C2-N1-C1'	7.39	126.57	117.70
34	BB	99	A	N3-C4-N9	7.38	133.30	127.40
33	BA	1352	U	C2-N1-C1'	7.37	126.55	117.70
1	AA	439	A	C5-N7-C8	7.34	107.57	103.90
33	BA	527	A	C4-C5-C6	7.34	120.67	117.00
1	AA	1167	C	C2-N1-C1'	7.33	126.86	118.80
33	BA	1433	U	C2-N1-C1'	7.32	126.49	117.70
33	BA	1188	A	C5-N7-C8	7.31	107.55	103.90
33	BA	935	A	C4-C5-C6	7.30	120.65	117.00
33	BA	2407	A	C4-C5-C6	7.28	120.64	117.00
33	BA	1067	A	C5-N7-C8	7.22	107.51	103.90
1	AA	1278	A	C4-C5-C6	7.21	120.61	117.00
1	AA	993	A	N3-C4-N9	7.20	133.16	127.40
33	BA	679	A	C4-C5-C6	7.18	120.59	117.00
1	AA	308	A	C4-C5-C6	7.17	120.58	117.00
33	BA	527	A	N3-C4-N9	7.17	133.13	127.40
1	AA	391	A	C4-C5-C6	7.15	120.58	117.00
1	AA	507	A	C5-C6-N1	7.14	121.27	117.70
33	BA	513	A	N3-C4-N9	7.12	133.10	127.40
1	AA	99	A	N3-C4-N9	7.12	133.09	127.40
33	BA	913	A	N3-C4-N9	7.12	133.09	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	405	A	C4-C5-C6	7.09	120.55	117.00
34	BB	99	A	C5-N7-C8	7.09	107.44	103.90
1	AA	572	A	N3-C4-N9	7.06	133.05	127.40
33	BA	1618	A	C4-C5-C6	7.05	120.53	117.00
33	BA	2786	A	N3-C4-N9	7.04	133.03	127.40
33	BA	1352	U	N1-C2-O2	7.03	127.72	122.80
33	BA	2691	A	C4-C5-C6	7.03	120.51	117.00
33	BA	1581	A	N3-C4-N9	6.97	132.97	127.40
33	BA	551	A	C4-C5-C6	6.96	120.48	117.00
33	BA	254	A	C4-C5-C6	6.96	120.48	117.00
33	BA	1691	A	C4-C5-C6	6.94	120.47	117.00
33	BA	732	A	C5-N7-C8	6.90	107.35	103.90
33	BA	559	A	C4-C5-C6	6.89	120.44	117.00
33	BA	935	A	N3-C4-N9	6.86	132.89	127.40
1	AA	1234	A	N3-C4-N9	6.86	132.89	127.40
33	BA	2202	A	N3-C4-N9	6.85	132.88	127.40
1	AA	1026	A	N3-C4-N9	6.85	132.88	127.40
1	AA	1167	C	N1-C2-O2	6.84	123.00	118.90
33	BA	52	A	C4-C5-C6	6.84	120.42	117.00
1	AA	1288	A	N3-C4-N9	6.83	132.87	127.40
33	BA	168	A	C4-C5-C6	6.83	120.42	117.00
1	AA	993	A	C4-C5-C6	6.83	120.41	117.00
33	BA	226	A	C4-C5-C6	6.82	120.41	117.00
33	BA	478	U	N1-C2-O2	6.81	127.57	122.80
21	AX	9	A	C4-C5-C6	6.81	120.41	117.00
33	BA	1433	U	N1-C2-O2	6.81	127.57	122.80
1	AA	1308	A	C4-C5-C6	6.80	120.40	117.00
1	AA	790	A	C4-C5-C6	6.79	120.40	117.00
33	BA	1714	A	C4-C5-C6	6.79	120.39	117.00
33	BA	1094	A	C4-C5-C6	6.78	120.39	117.00
1	AA	1427	A	C4-C5-C6	6.78	120.39	117.00
1	AA	99	A	C4-C5-C6	6.77	120.39	117.00
33	BA	2143	A	N3-C4-N9	6.77	132.81	127.40
33	BA	2735	A	N3-C4-N9	6.76	132.81	127.40
33	BA	2735	A	C4-C5-C6	6.76	120.38	117.00
33	BA	2111	A	C4-C5-C6	6.75	120.38	117.00
33	BA	661	A	C4-C5-C6	6.75	120.38	117.00
33	BA	2786	A	C4-C5-C6	6.75	120.38	117.00
33	BA	2627	A	N3-C4-N9	6.75	132.80	127.40
1	AA	1166	A	N3-C4-N9	6.75	132.80	127.40
33	BA	866	A	C4-C5-C6	6.75	120.37	117.00
1	AA	911	A	C4-C5-C6	6.73	120.37	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1883	A	C4-C5-C6	6.73	120.36	117.00
33	BA	2395	A	C4-C5-C6	6.73	120.36	117.00
33	BA	1667	A	N3-C4-N9	6.71	132.77	127.40
1	AA	308	A	N3-C4-N9	6.71	132.77	127.40
33	BA	736	A	N3-C4-N9	6.71	132.77	127.40
33	BA	2202	A	C4-C5-C6	6.70	120.35	117.00
1	AA	572	A	C4-C5-C6	6.70	120.35	117.00
33	BA	913	A	C4-C5-C6	6.70	120.35	117.00
33	BA	2176	A	C4-C5-C6	6.70	120.35	117.00
1	AA	1384	A	C4-C5-C6	6.69	120.35	117.00
33	BA	1839	A	C4-C5-C6	6.68	120.34	117.00
1	AA	195	A	N3-C4-N9	6.68	132.75	127.40
1	AA	987	A	N3-C4-N9	6.68	132.75	127.40
33	BA	2106	A	C4-C5-C6	6.68	120.34	117.00
33	BA	56	A	N3-C4-N9	6.68	132.74	127.40
33	BA	390	A	C4-C5-C6	6.68	120.34	117.00
33	BA	2459	A	C4-C5-C6	6.67	120.34	117.00
1	AA	1315	A	C4-C5-C6	6.67	120.34	117.00
33	BA	679	A	N3-C4-N9	6.67	132.73	127.40
1	AA	1065	A	C4-C5-C6	6.66	120.33	117.00
33	BA	2407	A	N3-C4-N9	6.66	132.73	127.40
33	BA	2043	A	C4-C5-C6	6.66	120.33	117.00
33	BA	1075	A	C4-C5-C6	6.65	120.33	117.00
33	BA	1667	A	C4-C5-C6	6.65	120.33	117.00
33	BA	1619	A	C4-C5-C6	6.65	120.32	117.00
1	AA	391	A	N3-C4-N9	6.65	132.72	127.40
33	BA	673	A	C4-C5-C6	6.65	120.32	117.00
33	BA	2844	A	C4-C5-C6	6.65	120.32	117.00
33	BA	390	A	N3-C4-N9	6.64	132.72	127.40
33	BA	752	A	C4-C5-C6	6.64	120.32	117.00
33	BA	2885	A	N3-C4-N9	6.63	132.71	127.40
33	BA	1831	A	C4-C5-C6	6.63	120.31	117.00
33	BA	2164	A	C4-C5-C6	6.62	120.31	117.00
33	BA	722	A	C4-C5-C6	6.62	120.31	117.00
33	BA	518	A	C4-C5-C6	6.62	120.31	117.00
33	BA	1816	A	N3-C4-N9	6.62	132.69	127.40
33	BA	2459	A	N3-C4-N9	6.62	132.69	127.40
33	BA	1006	A	N3-C4-N9	6.61	132.69	127.40
1	AA	727	A	N3-C4-N9	6.60	132.68	127.40
1	AA	933	A	C4-C5-C6	6.59	120.30	117.00
33	BA	1393	A	C4-C5-C6	6.58	120.29	117.00
33	BA	593	A	N3-C4-N9	6.58	132.66	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2691	A	N3-C4-N9	6.58	132.66	127.40
1	AA	1234	A	C4-C5-C6	6.58	120.29	117.00
33	BA	254	A	N3-C4-N9	6.57	132.66	127.40
33	BA	1398	A	N3-C4-N9	6.56	132.65	127.40
34	BB	97	A	C4-C5-C6	6.56	120.28	117.00
33	BA	538	A	C4-C5-C6	6.55	120.28	117.00
1	AA	337	A	C4-C5-C6	6.55	120.28	117.00
33	BA	948	A	N3-C4-N9	6.55	132.64	127.40
33	BA	501	A	C4-C5-N7	-6.54	107.43	110.70
33	BA	1999	A	C4-C5-C6	6.54	120.27	117.00
33	BA	2044	A	C4-C5-C6	6.54	120.27	117.00
1	AA	507	A	N3-C4-N9	6.54	132.63	127.40
1	AA	1166	A	C4-C5-C6	6.54	120.27	117.00
33	BA	2844	A	N3-C4-N9	6.54	132.63	127.40
1	AA	1341	A	N3-C4-N9	6.54	132.63	127.40
33	BA	2862	A	N3-C4-N9	6.54	132.63	127.40
1	AA	397	A	C4-C5-C6	6.53	120.27	117.00
1	AA	114	A	N3-C4-N9	6.53	132.62	127.40
1	AA	114	A	C4-C5-C6	6.53	120.26	117.00
33	BA	656	A	C4-C5-C6	6.53	120.26	117.00
33	BA	1442	A	N3-C4-N9	6.53	132.62	127.40
33	BA	1480	A	N3-C4-N9	6.53	132.62	127.40
33	BA	1778	A	C4-C5-C6	6.52	120.26	117.00
1	AA	508	A	N9-C4-C5	6.52	108.41	105.80
33	BA	1858	A	C4-C5-C6	6.52	120.26	117.00
33	BA	2862	A	C4-C5-C6	6.52	120.26	117.00
33	BA	1360	A	N3-C4-N9	6.51	132.61	127.40
33	BA	1433	U	N3-C2-O2	-6.51	117.64	122.20
34	BB	13	A	N3-C4-N9	6.51	132.61	127.40
33	BA	95	A	C4-C5-C6	6.51	120.26	117.00
33	BA	1103	A	N3-C4-N9	6.51	132.61	127.40
33	BA	1562	A	N3-C4-N9	6.51	132.61	127.40
1	AA	76	A	C4-C5-C6	6.51	120.25	117.00
33	BA	910	A	N3-C4-N9	6.51	132.61	127.40
1	AA	1133	A	N9-C4-C5	6.51	108.40	105.80
33	BA	108	A	C4-C5-C6	6.51	120.25	117.00
33	BA	108	A	N3-C4-N9	6.51	132.61	127.40
33	BA	258	A	C4-C5-C6	6.51	120.25	117.00
33	BA	559	A	N3-C4-N9	6.51	132.60	127.40
1	AA	335	A	C4-C5-C6	6.50	120.25	117.00
1	AA	1478	A	C4-C5-C6	6.50	120.25	117.00
33	BA	1073	A	N3-C4-N9	6.50	132.60	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1581	A	C4-C5-C6	6.50	120.25	117.00
33	BA	1653	A	C4-C5-C6	6.50	120.25	117.00
33	BA	634	A	C4-C5-C6	6.50	120.25	117.00
33	BA	95	A	N3-C4-N9	6.49	132.59	127.40
33	BA	1618	A	N3-C4-N9	6.49	132.59	127.40
33	BA	2143	A	C4-C5-C6	6.49	120.24	117.00
1	AA	1288	A	C4-C5-C6	6.49	120.24	117.00
33	BA	673	A	N3-C4-N9	6.49	132.59	127.40
33	BA	1562	A	C4-C5-C6	6.48	120.24	117.00
33	BA	2111	A	N3-C4-N9	6.48	132.59	127.40
33	BA	589	G	P-O3'-C3'	6.48	127.48	119.70
1	AA	1341	A	C4-C5-C6	6.48	120.24	117.00
33	BA	1638	A	N3-C4-N9	6.48	132.58	127.40
33	BA	1485	A	C4-C5-C6	6.47	120.24	117.00
33	BA	1816	A	C4-C5-C6	6.47	120.24	117.00
33	BA	2436	A	N3-C4-N9	6.47	132.58	127.40
33	BA	2205	A	C4-C5-C6	6.47	120.23	117.00
33	BA	2794	A	N3-C4-N9	6.47	132.57	127.40
33	BA	2339	A	N3-C4-N9	6.46	132.57	127.40
33	BA	1778	A	N3-C4-N9	6.46	132.57	127.40
33	BA	2123	A	C4-C5-C6	6.46	120.23	117.00
1	AA	649	A	N3-C4-N9	6.46	132.57	127.40
33	BA	736	A	C4-C5-C6	6.46	120.23	117.00
33	BA	1392	A	C4-C5-C6	6.46	120.23	117.00
33	BA	1491	A	N3-C4-N9	6.46	132.57	127.40
1	AA	57	A	C4-C5-C6	6.45	120.22	117.00
1	AA	397	A	N3-C4-N9	6.45	132.56	127.40
33	BA	2123	A	N3-C4-N9	6.45	132.56	127.40
33	BA	551	A	N3-C4-N9	6.44	132.55	127.40
33	BA	517	A	C4-C5-C6	6.44	120.22	117.00
33	BA	2163	A	N3-C4-N9	6.44	132.55	127.40
33	BA	2241	A	N9-C4-C5	6.44	108.38	105.80
33	BA	715	A	N3-C4-N9	6.44	132.55	127.40
33	BA	866	A	N3-C4-N9	6.43	132.55	127.40
33	BA	2689	A	N3-C4-N9	6.43	132.54	127.40
33	BA	501	A	N9-C4-C5	6.43	108.37	105.80
33	BA	2163	A	C4-C5-C6	6.43	120.21	117.00
33	BA	56	A	C4-C5-C6	6.42	120.21	117.00
1	AA	727	A	C4-C5-C6	6.42	120.21	117.00
33	BA	656	A	N3-C4-N9	6.42	132.53	127.40
33	BA	689	A	N3-C4-N9	6.42	132.53	127.40
33	BA	1820	A	C4-C5-C6	6.42	120.21	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2117	A	N3-C4-N9	6.42	132.53	127.40
33	BA	185	A	N3-C4-N9	6.42	132.53	127.40
1	AA	933	A	N3-C4-N9	6.41	132.53	127.40
33	BA	1096	A	C4-C5-C6	6.41	120.20	117.00
33	BA	1888	A	C4-C5-C6	6.41	120.21	117.00
33	BA	538	A	N3-C4-N9	6.41	132.53	127.40
33	BA	1999	A	N3-C4-N9	6.41	132.53	127.40
33	BA	2436	A	C4-C5-C6	6.41	120.20	117.00
33	BA	1094	A	N3-C4-N9	6.41	132.52	127.40
33	BA	1103	A	C4-C5-C6	6.40	120.20	117.00
33	BA	1485	A	N3-C4-N9	6.40	132.52	127.40
33	BA	2402	A	C4-C5-C6	6.40	120.20	117.00
33	BA	2805	A	C4-C5-C6	6.40	120.20	117.00
1	AA	918	A	C4-C5-C6	6.40	120.20	117.00
33	BA	2339	A	C4-C5-C6	6.40	120.20	117.00
1	AA	790	A	N3-C4-N9	6.40	132.52	127.40
1	AA	1442	A	C4-C5-C6	6.40	120.20	117.00
1	AA	649	A	C4-C5-C6	6.40	120.20	117.00
33	BA	634	A	N3-C4-N9	6.39	132.51	127.40
33	BA	1442	A	C4-C5-C6	6.39	120.20	117.00
33	BA	2794	A	C4-C5-C6	6.39	120.20	117.00
1	AA	987	A	C4-C5-C6	6.39	120.19	117.00
33	BA	1638	A	C4-C5-C6	6.39	120.19	117.00
33	BA	2532	A	N3-C4-N9	6.39	132.51	127.40
1	AA	948	A	C4-C5-C6	6.39	120.19	117.00
21	AX	24	A	N3-C4-N9	6.38	132.51	127.40
1	AA	1065	A	N3-C4-N9	6.38	132.50	127.40
33	BA	168	A	N3-C4-N9	6.38	132.50	127.40
1	AA	844	A	C4-C5-C6	6.38	120.19	117.00
33	BA	774	A	C8-N9-C4	6.38	108.35	105.80
33	BA	1900	A	N3-C4-N9	6.38	132.50	127.40
33	BA	2026	A	C4-C5-C6	6.38	120.19	117.00
33	BA	948	A	C4-C5-C6	6.38	120.19	117.00
34	BB	46	A	N3-C4-N9	6.38	132.50	127.40
33	BA	1352	U	N3-C2-O2	-6.37	117.74	122.20
33	BA	1536	A	N3-C4-N9	6.37	132.50	127.40
33	BA	1360	A	C4-C5-C6	6.37	120.19	117.00
1	AA	128	A	N3-C4-N9	6.37	132.50	127.40
1	AA	844	A	N3-C4-N9	6.37	132.49	127.40
1	AA	883	A	C4-C5-C6	6.36	120.18	117.00
1	AA	1143	A	N3-C4-N9	6.36	132.49	127.40
33	BA	1858	A	N3-C4-N9	6.36	132.49	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2827	A	C4-C5-C6	6.36	120.18	117.00
33	BA	259	A	C4-C5-C6	6.36	120.18	117.00
33	BA	752	A	N3-C4-N9	6.36	132.48	127.40
34	BB	13	A	C4-C5-C6	6.36	120.18	117.00
1	AA	1278	A	N3-C4-N9	6.35	132.48	127.40
1	AA	1517	A	N3-C4-N9	6.35	132.48	127.40
33	BA	2043	A	N3-C4-N9	6.35	132.48	127.40
33	BA	590	U	P-O5'-C5'	6.35	131.06	120.90
1	AA	1160	A	N3-C4-N9	6.35	132.48	127.40
33	BA	2027	A	C4-C5-C6	6.35	120.17	117.00
33	BA	90	A	C4-C5-C6	6.35	120.17	117.00
33	BA	2441	A	C4-C5-C6	6.35	120.17	117.00
33	BA	265	A	C4-C5-C6	6.35	120.17	117.00
33	BA	478	U	N3-C2-O2	-6.35	117.76	122.20
33	BA	2205	A	N3-C4-N9	6.35	132.48	127.40
34	BB	11	A	N3-C4-N9	6.35	132.48	127.40
33	BA	526	A	N9-C4-C5	6.34	108.34	105.80
33	BA	692	A	C4-C5-C6	6.34	120.17	117.00
33	BA	1709	A	C4-C5-C6	6.34	120.17	117.00
1	AA	337	A	N3-C4-N9	6.34	132.47	127.40
33	BA	715	A	C4-C5-C6	6.34	120.17	117.00
33	BA	661	A	N3-C4-N9	6.34	132.47	127.40
33	BA	2349	A	C4-C5-C6	6.34	120.17	117.00
33	BA	1258	A	N3-C4-N9	6.34	132.47	127.40
33	BA	2395	A	N3-C4-N9	6.34	132.47	127.40
33	BA	1253	A	C4-C5-C6	6.34	120.17	117.00
1	AA	1179	A	C4-C5-C6	6.33	120.17	117.00
1	AA	1493	A	C4-C5-C6	6.33	120.17	117.00
33	BA	1222	A	N3-C4-N9	6.33	132.47	127.40
1	AA	811	A	C4-C5-C6	6.33	120.17	117.00
33	BA	970	A	N3-C4-N9	6.33	132.47	127.40
33	BA	2790	A	N3-C4-N9	6.33	132.47	127.40
1	AA	1297	A	C4-C5-C6	6.33	120.17	117.00
33	BA	964	A	C4-C5-C6	6.33	120.17	117.00
33	BA	2117	A	C4-C5-C6	6.33	120.17	117.00
33	BA	1506	A	N3-C4-N9	6.33	132.46	127.40
33	BA	1877	A	C4-C5-C6	6.33	120.16	117.00
1	AA	161	A	C4-C5-C6	6.32	120.16	117.00
33	BA	689	A	C4-C5-C6	6.32	120.16	117.00
33	BA	1019	A	C4-C5-C6	6.32	120.16	117.00
33	BA	2402	A	N3-C4-N9	6.32	132.46	127.40
1	AA	1272	A	N3-C4-N9	6.32	132.46	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AX	9	A	N3-C4-N9	6.32	132.46	127.40
33	BA	1839	A	N3-C4-N9	6.32	132.46	127.40
33	BA	1998	A	C4-C5-C6	6.32	120.16	117.00
33	BA	2358	A	C4-C5-C6	6.32	120.16	117.00
33	BA	2689	A	C4-C5-C6	6.32	120.16	117.00
33	BA	2106	A	N3-C4-N9	6.31	132.45	127.40
1	AA	911	A	N3-C4-N9	6.31	132.45	127.40
1	AA	1155	A	C4-C5-C6	6.31	120.16	117.00
33	BA	732	A	N3-C4-N9	6.31	132.45	127.40
33	BA	2694	A	C4-C5-C6	6.31	120.16	117.00
1	AA	1256	A	C4-C5-C6	6.31	120.16	117.00
1	AA	996	A	C4-C5-C6	6.31	120.16	117.00
1	AA	1372	A	N9-C4-C5	6.31	108.32	105.80
33	BA	1258	A	C4-C5-C6	6.31	120.15	117.00
33	BA	2100	A	C4-C5-C6	6.31	120.15	117.00
1	AA	74	A	C4-C5-C6	6.31	120.15	117.00
1	AA	1315	A	N3-C4-N9	6.31	132.44	127.40
21	AX	24	A	C4-C5-C6	6.30	120.15	117.00
33	BA	38	A	C4-C5-C6	6.30	120.15	117.00
33	BA	690	A	C4-C5-C6	6.30	120.15	117.00
33	BA	1776	A	N3-C4-N9	6.30	132.44	127.40
1	AA	838	A	N3-C4-N9	6.30	132.44	127.40
33	BA	1710	A	C4-C5-C6	6.30	120.15	117.00
33	BA	2517	A	C4-C5-C6	6.30	120.15	117.00
1	AA	76	A	N3-C4-N9	6.30	132.44	127.40
1	AA	743	A	C4-C5-C6	6.30	120.15	117.00
33	BA	2329	A	N3-C4-N9	6.30	132.44	127.40
33	BA	2329	A	C4-C5-C6	6.30	120.15	117.00
33	BA	2351	A	C4-C5-C6	6.30	120.15	117.00
33	BA	910	A	C4-C5-C6	6.30	120.15	117.00
33	BA	1877	A	N3-C4-N9	6.30	132.44	127.40
33	BA	1620	A	C4-C5-C6	6.29	120.15	117.00
33	BA	1480	A	C4-C5-C6	6.29	120.15	117.00
33	BA	1653	A	N3-C4-N9	6.29	132.44	127.40
33	BA	2349	A	N3-C4-N9	6.29	132.44	127.40
33	BA	2812	A	C4-C5-C6	6.29	120.15	117.00
33	BA	2831	A	C4-C5-C6	6.29	120.15	117.00
34	BB	46	A	C4-C5-C6	6.29	120.14	117.00
33	BA	117	A	C4-C5-C6	6.29	120.14	117.00
33	BA	258	A	N3-C4-N9	6.29	132.43	127.40
33	BA	1222	A	C4-C5-C6	6.29	120.14	117.00
33	BA	90	A	N3-C4-N9	6.29	132.43	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	193	A	C4-C5-C6	6.29	120.14	117.00
33	BA	1745	A	C4-C5-C6	6.29	120.14	117.00
1	AA	705	A	C4-C5-C6	6.28	120.14	117.00
1	AA	948	A	N3-C4-N9	6.28	132.43	127.40
33	BA	2026	A	N3-C4-N9	6.28	132.42	127.40
33	BA	974	A	C4-C5-C6	6.28	120.14	117.00
33	BA	1190	A	C4-C5-C6	6.28	120.14	117.00
34	BB	11	A	C4-C5-C6	6.28	120.14	117.00
33	BA	1392	A	N3-C4-N9	6.28	132.42	127.40
33	BA	724	A	N3-C4-N9	6.28	132.42	127.40
33	BA	1820	A	N3-C4-N9	6.28	132.42	127.40
33	BA	2812	A	N3-C4-N9	6.28	132.42	127.40
1	AA	1384	A	N3-C4-N9	6.27	132.42	127.40
33	BA	437	A	N3-C4-N9	6.27	132.42	127.40
33	BA	2616	A	C4-C5-C6	6.27	120.14	117.00
33	BA	438	A	N3-C4-N9	6.27	132.42	127.40
33	BA	496	A	N3-C4-N9	6.27	132.42	127.40
33	BA	1885	A	C4-C5-C6	6.27	120.14	117.00
1	AA	875	A	N3-C4-N9	6.27	132.41	127.40
1	AA	882	A	C4-C5-C6	6.27	120.14	117.00
1	AA	1143	A	C4-C5-C6	6.27	120.13	117.00
1	AA	1256	A	N3-C4-N9	6.27	132.41	127.40
33	BA	1073	A	C4-C5-C6	6.27	120.14	117.00
33	BA	1709	A	N3-C4-N9	6.27	132.42	127.40
1	AA	1272	A	C4-C5-C6	6.27	120.13	117.00
33	BA	630	A	C4-C5-C6	6.27	120.13	117.00
33	BA	1883	A	N3-C4-N9	6.27	132.41	127.40
33	BA	1536	A	C4-C5-C6	6.27	120.13	117.00
33	BA	1895	A	C4-C5-C6	6.27	120.13	117.00
1	AA	335	A	N3-C4-N9	6.26	132.41	127.40
33	BA	1096	A	N3-C4-N9	6.26	132.41	127.40
1	AA	1478	A	N3-C4-N9	6.26	132.41	127.40
33	BA	275	A	C4-C5-C6	6.26	120.13	117.00
1	AA	1238	A	C4-C5-C6	6.26	120.13	117.00
33	BA	549	A	C4-C5-C6	6.26	120.13	117.00
33	BA	2343	A	C4-C5-C6	6.26	120.13	117.00
33	BA	130	A	C4-C5-C6	6.26	120.13	117.00
33	BA	1695	A	C4-C5-C6	6.26	120.13	117.00
33	BA	1945	A	C4-C5-C6	6.26	120.13	117.00
33	BA	1490	A	C4-C5-C6	6.26	120.13	117.00
33	BA	1235	A	C4-C5-C6	6.26	120.13	117.00
33	BA	1768	A	C4-C5-C6	6.26	120.13	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2790	A	C4-C5-C6	6.26	120.13	117.00
33	BA	943	A	C4-C5-C6	6.25	120.13	117.00
33	BA	2358	A	N3-C4-N9	6.25	132.40	127.40
1	AA	674	A	N9-C4-C5	6.25	108.30	105.80
1	AA	1133	A	C4-C5-N7	-6.25	107.57	110.70
1	AA	1383	A	C4-C5-C6	6.25	120.13	117.00
33	BA	956	A	C4-C5-C6	6.25	120.13	117.00
1	AA	882	A	N3-C4-N9	6.25	132.40	127.40
1	AA	917	A	C4-C5-C6	6.25	120.12	117.00
33	BA	678	A	C4-C5-C6	6.25	120.12	117.00
33	BA	1831	A	N3-C4-N9	6.25	132.40	127.40
1	AA	1155	A	N3-C4-N9	6.25	132.40	127.40
33	BA	1710	A	N3-C4-N9	6.25	132.40	127.40
33	BA	2916	A	N9-C4-C5	6.25	108.30	105.80
33	BA	2027	A	N3-C4-N9	6.25	132.40	127.40
1	AA	1517	A	C4-C5-C6	6.25	120.12	117.00
33	BA	1316	A	N3-C4-N9	6.25	132.40	127.40
1	AA	838	A	C4-C5-C6	6.24	120.12	117.00
1	AA	984	A	C4-C5-C6	6.24	120.12	117.00
33	BA	790	A	C4-C5-C6	6.24	120.12	117.00
33	BA	1126	A	N3-C4-N9	6.24	132.40	127.40
33	BA	1900	A	C4-C5-C6	6.24	120.12	117.00
33	BA	2049	A	C4-C5-C6	6.24	120.12	117.00
33	BA	2662	A	C4-C5-C6	6.24	120.12	117.00
33	BA	2662	A	N3-C4-N9	6.24	132.40	127.40
33	BA	578	A	N3-C4-N9	6.24	132.39	127.40
33	BA	2464	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1222	A	C4-C5-C6	6.24	120.12	117.00
33	BA	2241	A	C4-C5-N7	-6.24	107.58	110.70
1	AA	1112	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1427	A	N3-C4-N9	6.24	132.39	127.40
33	BA	2365	A	N3-C4-N9	6.24	132.39	127.40
33	BA	456	A	C4-C5-C6	6.24	120.12	117.00
33	BA	462	A	C4-C5-C6	6.24	120.12	117.00
33	BA	1776	A	C4-C5-C6	6.24	120.12	117.00
33	BA	2381	A	C4-C5-C6	6.24	120.12	117.00
33	BA	1655	A	C4-C5-C6	6.23	120.12	117.00
33	BA	130	A	N3-C4-N9	6.23	132.39	127.40
33	BA	578	A	C4-C5-C6	6.23	120.12	117.00
33	BA	2924	A	C4-C5-C6	6.23	120.12	117.00
33	BA	376	A	C4-C5-C6	6.23	120.11	117.00
1	AA	1160	A	C4-C5-C6	6.23	120.11	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AX	70	A	C4-C5-C6	6.23	120.11	117.00
33	BA	133	A	N3-C4-N9	6.23	132.38	127.40
33	BA	391	A	C4-C5-C6	6.23	120.11	117.00
33	BA	1727	A	C4-C5-C6	6.23	120.11	117.00
1	AA	548	A	C4-C5-C6	6.22	120.11	117.00
33	BA	1490	A	N3-C4-N9	6.22	132.38	127.40
33	BA	1575	A	C4-C5-C6	6.22	120.11	117.00
1	AA	996	A	N3-C4-N9	6.22	132.38	127.40
33	BA	2629	A	C4-C5-C6	6.22	120.11	117.00
33	BA	2805	A	C8-N9-C4	6.22	108.29	105.80
1	AA	715	A	C4-C5-C6	6.22	120.11	117.00
1	AA	74	A	N3-C4-N9	6.22	132.38	127.40
1	AA	1016	A	C4-C5-C6	6.22	120.11	117.00
33	BA	1901	A	C4-C5-C6	6.22	120.11	117.00
1	AA	57	A	N3-C4-N9	6.22	132.37	127.40
34	BB	97	A	N3-C4-N9	6.22	132.37	127.40
1	AA	711	A	N3-C4-N9	6.21	132.37	127.40
33	BA	2532	A	C4-C5-C6	6.21	120.11	117.00
33	BA	496	A	C4-C5-C6	6.21	120.11	117.00
33	BA	2176	A	N3-C4-N9	6.21	132.37	127.40
33	BA	52	A	N3-C4-N9	6.21	132.37	127.40
33	BA	1190	A	N3-C4-N9	6.21	132.37	127.40
33	BA	722	A	N3-C4-N9	6.21	132.37	127.40
33	BA	943	A	N3-C4-N9	6.21	132.37	127.40
1	AA	548	A	N3-C4-N9	6.21	132.36	127.40
1	AA	711	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1189	A	C4-C5-C6	6.20	120.10	117.00
33	BA	724	A	C4-C5-C6	6.20	120.10	117.00
33	BA	1426	A	C4-C5-C6	6.20	120.10	117.00
33	BA	1672	A	N3-C4-N9	6.20	132.36	127.40
33	BA	2270	A	C4-C5-C6	6.20	120.10	117.00
33	BA	592	A	C4-C5-C6	6.20	120.10	117.00
33	BA	870	A	N3-C4-N9	6.20	132.36	127.40
33	BA	2663	A	N3-C4-N9	6.20	132.36	127.40
33	BA	1845	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1442	A	N3-C4-N9	6.20	132.36	127.40
1	AA	128	A	C4-C5-C6	6.20	120.10	117.00
33	BA	1075	A	N3-C4-N9	6.20	132.36	127.40
33	BA	194	A	C4-C5-C6	6.20	120.10	117.00
33	BA	326	A	C4-C5-C6	6.20	120.10	117.00
33	BA	343	A	C4-C5-C6	6.20	120.10	117.00
33	BA	699	A	C4-C5-C6	6.20	120.10	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2365	A	C4-C5-C6	6.20	120.10	117.00
33	BA	1067	A	N9-C4-C5	6.19	108.28	105.80
33	BA	1461	A	C4-C5-C6	6.19	120.10	117.00
33	BA	2848	A	C4-C5-C6	6.19	120.10	117.00
33	BA	690	A	N3-C4-N9	6.19	132.35	127.40
33	BA	882	A	N3-C4-N9	6.19	132.35	127.40
33	BA	1724	A	C4-C5-C6	6.19	120.09	117.00
1	AA	173	A	C4-C5-C6	6.19	120.09	117.00
1	AA	555	A	C4-C5-C6	6.19	120.09	117.00
1	AA	1366	A	C4-C5-C6	6.19	120.09	117.00
33	BA	518	A	N3-C4-N9	6.19	132.35	127.40
33	BA	1316	A	C4-C5-C6	6.19	120.09	117.00
33	BA	1686	A	C4-C5-C6	6.19	120.09	117.00
33	BA	2919	A	C4-C5-C6	6.19	120.09	117.00
1	AA	617	A	C4-C5-C6	6.19	120.09	117.00
33	BA	616	A	C4-C5-C6	6.19	120.09	117.00
33	BA	2200	A	C4-C5-C6	6.19	120.09	117.00
1	AA	875	A	C4-C5-C6	6.18	120.09	117.00
33	BA	1714	A	C5-C6-N1	6.18	120.79	117.70
33	BA	2302	A	C4-C5-C6	6.18	120.09	117.00
33	BA	2351	A	N3-C4-N9	6.18	132.35	127.40
33	BA	2252	A	C4-C5-C6	6.18	120.09	117.00
1	AA	1004	A	N3-C4-N9	6.18	132.34	127.40
33	BA	1132	A	N3-C4-N9	6.18	132.34	127.40
33	BA	1569	A	C4-C5-C6	6.18	120.09	117.00
1	AA	282	A	C4-C5-C6	6.18	120.09	117.00
1	AA	605	A	N3-C4-N9	6.18	132.34	127.40
33	BA	133	A	C4-C5-C6	6.18	120.09	117.00
33	BA	260	A	C4-C5-C6	6.18	120.09	117.00
33	BA	1286	A	N3-C4-N9	6.18	132.34	127.40
33	BA	1655	A	N3-C4-N9	6.18	132.34	127.40
33	BA	2148	A	C4-C5-C6	6.18	120.09	117.00
33	BA	407	A	C4-C5-C6	6.18	120.09	117.00
1	AA	617	A	N3-C4-N9	6.18	132.34	127.40
1	AA	1016	A	N3-C4-N9	6.18	132.34	127.40
33	BA	692	A	N3-C4-N9	6.18	132.34	127.40
1	AA	956	A	C4-C5-C6	6.17	120.09	117.00
33	BA	156	A	N3-C4-N9	6.17	132.34	127.40
33	BA	1100	A	C4-C5-C6	6.17	120.09	117.00
33	BA	1520	A	N3-C4-N9	6.17	132.34	127.40
33	BA	2316	A	C4-C5-C6	6.17	120.09	117.00
33	BA	2500	A	C4-C5-C6	6.17	120.09	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	171	A	N3-C4-N9	6.17	132.34	127.40
33	BA	1393	A	N3-C4-N9	6.17	132.34	127.40
33	BA	1556	A	C4-C5-C6	6.17	120.09	117.00
33	BA	1680	A	C4-C5-C6	6.17	120.09	117.00
1	AA	140	A	C4-C5-C6	6.17	120.09	117.00
1	AA	945	A	C4-C5-C6	6.17	120.09	117.00
33	BA	2694	A	N3-C4-N9	6.17	132.34	127.40
1	AA	721	A	C4-C5-C6	6.17	120.08	117.00
33	BA	61	A	N3-C4-N9	6.17	132.34	127.40
33	BA	517	A	N3-C4-N9	6.17	132.34	127.40
1	AA	55	A	C4-C5-C6	6.17	120.08	117.00
21	AX	37	A	N9-C4-C5	6.17	108.27	105.80
33	BA	353	A	C4-C5-C6	6.17	120.08	117.00
33	BA	956	A	N3-C4-N9	6.17	132.34	127.40
33	BA	1619	A	N3-C4-N9	6.17	132.34	127.40
33	BA	1695	A	N3-C4-N9	6.17	132.34	127.40
33	BA	2044	A	N3-C4-N9	6.17	132.34	127.40
33	BA	2700	A	C4-C5-C6	6.17	120.08	117.00
1	AA	72	A	C4-C5-C6	6.17	120.08	117.00
1	AA	301	A	N3-C4-N9	6.17	132.33	127.40
33	BA	1524	A	N3-C4-N9	6.17	132.33	127.40
33	BA	44	A	C4-C5-C6	6.16	120.08	117.00
33	BA	462	A	N3-C4-N9	6.16	132.33	127.40
33	BA	970	A	C4-C5-C6	6.16	120.08	117.00
1	AA	34	A	C4-C5-C6	6.16	120.08	117.00
33	BA	2164	A	N3-C4-N9	6.16	132.33	127.40
33	BA	2343	A	N3-C4-N9	6.16	132.33	127.40
33	BA	2570	A	C4-C5-C6	6.16	120.08	117.00
1	AA	282	A	N3-C4-N9	6.16	132.33	127.40
1	AA	959	A	C4-C5-C6	6.16	120.08	117.00
33	BA	574	A	N3-C4-N9	6.16	132.33	127.40
33	BA	2228	A	C4-C5-C6	6.16	120.08	117.00
33	BA	2722	A	C4-C5-C6	6.16	120.08	117.00
1	AA	496	A	C4-C5-C6	6.16	120.08	117.00
33	BA	185	A	C4-C5-C6	6.16	120.08	117.00
1	AA	956	A	N3-C4-N9	6.16	132.32	127.40
1	AA	1179	A	N3-C4-N9	6.16	132.32	127.40
1	AA	1425	A	C4-C5-C6	6.16	120.08	117.00
33	BA	1885	A	N3-C4-N9	6.16	132.32	127.40
33	BA	2052	A	C4-C5-C6	6.16	120.08	117.00
33	BA	1888	A	N3-C4-N9	6.15	132.32	127.40
1	AA	758	A	N3-C4-N9	6.15	132.32	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	61	A	C4-C5-C6	6.15	120.08	117.00
33	BA	156	A	C4-C5-C6	6.15	120.08	117.00
33	BA	1019	A	N3-C4-N9	6.15	132.32	127.40
33	BA	1620	A	N3-C4-N9	6.15	132.32	127.40
33	BA	2663	A	C4-C5-C6	6.15	120.08	117.00
33	BA	41	A	C4-C5-C6	6.15	120.08	117.00
33	BA	849	A	N3-C4-N9	6.15	132.32	127.40
1	AA	72	A	N3-C4-N9	6.14	132.31	127.40
21	AX	58	A	C4-C5-C6	6.14	120.07	117.00
21	AX	76	A	C4-C5-C6	6.14	120.07	117.00
33	BA	12	A	C4-C5-C6	6.14	120.07	117.00
33	BA	530	A	C4-C5-C6	6.14	120.07	117.00
33	BA	623	A	C4-C5-C6	6.14	120.07	117.00
33	BA	1056	A	C4-C5-C6	6.14	120.07	117.00
33	BA	1426	A	N3-C4-N9	6.14	132.32	127.40
33	BA	1882	A	C4-C5-C6	6.14	120.07	117.00
1	AA	55	A	N3-C4-N9	6.14	132.31	127.40
33	BA	140	A	C4-C5-C6	6.14	120.07	117.00
33	BA	431	A	C4-C5-C6	6.14	120.07	117.00
33	BA	889	A	C4-C5-C6	6.14	120.07	117.00
33	BA	1700	A	N3-C4-N9	6.14	132.31	127.40
1	AA	793	A	C4-C5-C6	6.14	120.07	117.00
33	BA	230	A	C4-C5-C6	6.14	120.07	117.00
33	BA	1357	A	N3-C4-N9	6.14	132.31	127.40
33	BA	1614	A	N3-C4-N9	6.14	132.31	127.40
1	AA	913	A	C4-C5-C6	6.14	120.07	117.00
33	BA	265	A	N3-C4-N9	6.14	132.31	127.40
33	BA	2500	A	N3-C4-N9	6.14	132.31	127.40
1	AA	918	A	N3-C4-N9	6.13	132.31	127.40
33	BA	560	A	N3-C4-N9	6.13	132.31	127.40
33	BA	1253	A	N3-C4-N9	6.13	132.31	127.40
33	BA	1357	A	C4-C5-C6	6.13	120.07	117.00
33	BA	1506	A	C4-C5-C6	6.13	120.07	117.00
33	BA	2846	A	C4-C5-C6	6.13	120.07	117.00
33	BA	1100	A	N3-C4-N9	6.13	132.31	127.40
33	BA	2200	A	N3-C4-N9	6.13	132.31	127.40
33	BA	971	A	C4-C5-C6	6.13	120.07	117.00
33	BA	1194	A	N3-C4-N9	6.13	132.31	127.40
33	BA	1491	A	C4-C5-C6	6.13	120.07	117.00
33	BA	1541	A	C4-C5-C6	6.13	120.07	117.00
33	BA	1768	A	N3-C4-N9	6.13	132.31	127.40
33	BA	1998	A	N3-C4-N9	6.13	132.31	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2560	A	C4-C5-C6	6.13	120.06	117.00
1	AA	1490	A	C4-C5-C6	6.13	120.06	117.00
33	BA	896	A	C4-C5-C6	6.13	120.06	117.00
33	BA	1286	A	C4-C5-C6	6.13	120.06	117.00
1	AA	902	A	C4-C5-C6	6.13	120.06	117.00
33	BA	530	A	N3-C4-N9	6.13	132.30	127.40
33	BA	1477	A	C4-C5-C6	6.13	120.06	117.00
33	BA	1767	A	C4-C5-C6	6.13	120.06	117.00
33	BA	2302	A	N3-C4-N9	6.13	132.30	127.40
33	BA	2826	A	N3-C4-N9	6.13	132.30	127.40
33	BA	2831	A	N3-C4-N9	6.13	132.30	127.40
1	AA	518	A	C4-C5-C6	6.13	120.06	117.00
33	BA	38	A	N3-C4-N9	6.13	132.30	127.40
33	BA	1721	A	C4-C5-C6	6.13	120.06	117.00
33	BA	2722	A	N3-C4-N9	6.13	132.30	127.40
1	AA	630	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1112	A	N3-C4-N9	6.12	132.30	127.40
1	AA	1283	A	C4-C5-C6	6.12	120.06	117.00
1	AA	433	A	C4-C5-C6	6.12	120.06	117.00
33	BA	593	A	C4-C5-C6	6.12	120.06	117.00
33	BA	1675	A	C4-C5-C6	6.12	120.06	117.00
33	BA	1947	A	C4-C5-C6	6.12	120.06	117.00
33	BA	2704	A	C4-C5-C6	6.12	120.06	117.00
33	BA	2900	A	C4-C5-C6	6.12	120.06	117.00
1	AA	278	A	N3-C4-N9	6.12	132.30	127.40
1	AA	883	A	N3-C4-N9	6.12	132.30	127.40
1	AA	1236	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1463	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1490	A	N3-C4-N9	6.12	132.30	127.40
33	BA	429	A	C4-C5-C6	6.12	120.06	117.00
33	BA	616	A	N3-C4-N9	6.12	132.30	127.40
33	BA	882	A	C4-C5-C6	6.12	120.06	117.00
33	BA	2270	A	N3-C4-N9	6.12	132.30	127.40
33	BA	2848	A	N3-C4-N9	6.12	132.30	127.40
1	AA	140	A	N3-C4-N9	6.12	132.30	127.40
1	AA	270	A	C4-C5-C6	6.12	120.06	117.00
1	AA	743	A	N3-C4-N9	6.12	132.30	127.40
33	BA	431	A	N3-C4-N9	6.12	132.30	127.40
33	BA	469	A	C4-C5-C6	6.12	120.06	117.00
33	BA	889	A	N3-C4-N9	6.12	132.29	127.40
33	BA	1398	A	C4-C5-C6	6.12	120.06	117.00
33	BA	1614	A	C4-C5-C6	6.12	120.06	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2080	A	C4-C5-C6	6.12	120.06	117.00
33	BA	1210	A	C4-C5-C6	6.12	120.06	117.00
1	AA	721	A	N3-C4-N9	6.12	132.29	127.40
1	AA	758	A	C4-C5-C6	6.12	120.06	117.00
1	AA	984	A	N3-C4-N9	6.12	132.29	127.40
1	AA	1004	A	C4-C5-C6	6.12	120.06	117.00
1	AA	1349	A	C4-C5-C6	6.12	120.06	117.00
1	AA	696	A	C4-C5-C6	6.11	120.06	117.00
33	BA	1957	A	C4-C5-C6	6.11	120.06	117.00
33	BA	391	A	N3-C4-N9	6.11	132.29	127.40
33	BA	592	A	N3-C4-N9	6.11	132.29	127.40
1	AA	1348	A	C4-C5-C6	6.11	120.06	117.00
33	BA	305	A	N3-C4-N9	6.11	132.29	127.40
33	BA	407	A	N3-C4-N9	6.11	132.29	127.40
33	BA	537	A	C4-C5-C6	6.11	120.06	117.00
33	BA	1848	A	C4-C5-C6	6.11	120.06	117.00
33	BA	2805	A	N3-C4-N9	6.11	132.29	127.40
1	AA	1161	A	C4-C5-C6	6.11	120.06	117.00
1	AA	99	A	C5-C6-N1	6.11	120.75	117.70
1	AA	346	A	C4-C5-C6	6.11	120.05	117.00
1	AA	1369	A	N3-C4-N9	6.11	132.29	127.40
33	BA	437	A	C4-C5-C6	6.11	120.05	117.00
33	BA	2105	U	C2-N1-C1'	6.11	125.03	117.70
33	BA	2560	A	N3-C4-N9	6.11	132.29	127.40
34	BB	20	A	C4-C5-C6	6.11	120.05	117.00
1	AA	301	A	C4-C5-C6	6.11	120.05	117.00
33	BA	765	A	C4-C5-C6	6.11	120.05	117.00
33	BA	1059	A	C4-C5-C6	6.11	120.05	117.00
33	BA	1995	A	C4-C5-C6	6.11	120.05	117.00
33	BA	2754	A	N3-C4-N9	6.11	132.28	127.40
33	BA	220	A	C4-C5-C6	6.10	120.05	117.00
33	BA	870	A	C4-C5-C6	6.10	120.05	117.00
33	BA	1477	A	N3-C4-N9	6.10	132.28	127.40
33	BA	2078	A	C4-C5-C6	6.10	120.05	117.00
1	AA	129	A	N3-C4-N9	6.10	132.28	127.40
1	AA	1024	A	C4-C5-C6	6.10	120.05	117.00
33	BA	326	A	N3-C4-N9	6.10	132.28	127.40
33	BA	549	A	N3-C4-N9	6.10	132.28	127.40
33	BA	1424	A	N3-C4-N9	6.10	132.28	127.40
33	BA	1524	A	C4-C5-C6	6.10	120.05	117.00
1	AA	234	A	C4-C5-C6	6.10	120.05	117.00
1	AA	969	A	C4-C5-C6	6.10	120.05	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	21	A	C4-C5-C6	6.10	120.05	117.00
34	BB	105	A	C4-C5-C6	6.10	120.05	117.00
1	AA	811	A	N3-C4-N9	6.10	132.28	127.40
1	AA	1284	A	C4-C5-C6	6.10	120.05	117.00
21	AX	70	A	N3-C4-N9	6.10	132.28	127.40
33	BA	193	A	N3-C4-N9	6.10	132.28	127.40
33	BA	456	A	N3-C4-N9	6.10	132.28	127.40
33	BA	868	A	C4-C5-C6	6.10	120.05	117.00
33	BA	1346	A	C4-C5-C6	6.10	120.05	117.00
33	BA	1636	A	C4-C5-C6	6.10	120.05	117.00
1	AA	433	A	N3-C4-N9	6.10	132.28	127.40
1	AA	659	A	N3-C4-N9	6.10	132.28	127.40
1	AA	862	A	N9-C4-C5	6.10	108.24	105.80
1	AA	1405	A	C4-C5-C6	6.10	120.05	117.00
33	BA	353	A	N3-C4-N9	6.10	132.28	127.40
33	BA	2511	A	C4-C5-C6	6.10	120.05	117.00
33	BA	2619	A	C4-C5-C6	6.10	120.05	117.00
33	BA	2854	A	C4-C5-C6	6.10	120.05	117.00
1	AA	1294	A	C4-C5-C6	6.10	120.05	117.00
1	AA	1486	A	C4-C5-C6	6.10	120.05	117.00
33	BA	21	A	N3-C4-N9	6.10	132.28	127.40
33	BA	1047	A	C4-C5-C6	6.10	120.05	117.00
1	AA	512	A	N3-C4-N9	6.09	132.28	127.40
33	BA	459	A	C4-C5-C6	6.09	120.05	117.00
33	BA	486	A	N3-C4-N9	6.09	132.28	127.40
33	BA	952	A	N3-C4-N9	6.09	132.28	127.40
33	BA	1005	A	C4-C5-C6	6.09	120.05	117.00
33	BA	2405	A	C4-C5-C6	6.09	120.05	117.00
33	BA	2517	A	N3-C4-N9	6.09	132.28	127.40
34	BB	50	A	C4-C5-C6	6.09	120.05	117.00
1	AA	803	A	C4-C5-C6	6.09	120.05	117.00
33	BA	41	A	N3-C4-N9	6.09	132.27	127.40
1	AA	913	A	N3-C4-N9	6.09	132.27	127.40
1	AA	1369	A	C4-C5-C6	6.09	120.05	117.00
33	BA	318	A	C4-C5-C6	6.09	120.05	117.00
33	BA	647	A	C8-N9-C4	6.09	108.24	105.80
33	BA	896	A	N3-C4-N9	6.09	132.27	127.40
33	BA	2052	A	N3-C4-N9	6.09	132.27	127.40
33	BA	2369	A	N3-C4-N9	6.09	132.27	127.40
1	AA	129	A	C4-C5-C6	6.09	120.04	117.00
1	AA	945	A	N3-C4-N9	6.09	132.27	127.40
1	AA	1252	A	C4-C5-C6	6.09	120.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1388	A	C4-C5-C6	6.09	120.05	117.00
33	BA	2170	A	C4-C5-C6	6.09	120.05	117.00
33	BA	2441	A	N3-C4-N9	6.09	132.27	127.40
33	BA	2779	A	C4-C5-C6	6.09	120.05	117.00
33	BA	964	A	N3-C4-N9	6.09	132.27	127.40
33	BA	2227	A	C4-C5-C6	6.09	120.04	117.00
1	AA	346	A	N3-C4-N9	6.09	132.27	127.40
1	AA	679	A	C4-C5-C6	6.09	120.04	117.00
33	BA	1901	A	N3-C4-N9	6.09	132.27	127.40
33	BA	2080	A	N3-C4-N9	6.09	132.27	127.40
33	BA	2826	A	C4-C5-C6	6.09	120.04	117.00
33	BA	525	A	C8-N9-C4	6.08	108.23	105.80
33	BA	1054	A	C4-C5-C6	6.08	120.04	117.00
1	AA	225	A	C4-C5-C6	6.08	120.04	117.00
1	AA	605	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1238	A	N3-C4-N9	6.08	132.27	127.40
1	AA	1245	A	N3-C4-N9	6.08	132.27	127.40
1	AA	1435	A	C4-C5-C6	6.08	120.04	117.00
33	BA	851	A	C4-C5-C6	6.08	120.04	117.00
33	BA	1265	A	C4-C5-C6	6.08	120.04	117.00
33	BA	1445	A	C4-C5-C6	6.08	120.04	117.00
33	BA	2297	A	C4-C5-C6	6.08	120.04	117.00
33	BA	2497	A	C4-C5-C6	6.08	120.04	117.00
34	BB	37	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1140	A	C4-C5-C6	6.08	120.04	117.00
33	BA	1421	A	C4-C5-C6	6.08	120.04	117.00
33	BA	1727	A	N3-C4-N9	6.08	132.26	127.40
33	BA	2220	A	C4-C5-C6	6.08	120.04	117.00
33	BA	2454	A	C4-C5-C6	6.08	120.04	117.00
33	BA	2488	A	C5'-C4'-C3'	-6.08	106.27	116.00
1	AA	671	A	N3-C4-N9	6.08	132.26	127.40
21	AX	21	A	C4-C5-C6	6.08	120.04	117.00
33	BA	1845	A	N3-C4-N9	6.08	132.26	127.40
1	AA	1405	A	N3-C4-N9	6.08	132.26	127.40
33	BA	91	A	C4-C5-C6	6.08	120.04	117.00
33	BA	1956	A	C4-C5-C6	6.08	120.04	117.00
33	BA	2252	A	N3-C4-N9	6.08	132.26	127.40
33	BA	2327	A	C4-C5-C6	6.08	120.04	117.00
33	BA	2387	A	C4-C5-C6	6.08	120.04	117.00
1	AA	404	A	C4-C5-C6	6.08	120.04	117.00
33	BA	144	A	C4-C5-C6	6.08	120.04	117.00
33	BA	2547	A	C4-C5-C6	6.08	120.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	374	A	N9-C4-C5	6.08	108.23	105.80
33	BA	1008	A	C4-C5-C6	6.08	120.04	117.00
33	BA	2369	A	C4-C5-C6	6.08	120.04	117.00
1	AA	161	A	N3-C4-N9	6.07	132.26	127.40
1	AA	671	A	C4-C5-C6	6.07	120.04	117.00
1	AA	1189	A	N3-C4-N9	6.07	132.26	127.40
1	AA	1297	A	N3-C4-N9	6.07	132.26	127.40
1	AA	1349	A	N3-C4-N9	6.07	132.26	127.40
1	AA	1437	A	C4-C5-C6	6.07	120.04	117.00
33	BA	73	A	C4-C5-C6	6.07	120.04	117.00
33	BA	589	G	C2'-C3'-O3'	-6.07	96.14	109.50
33	BA	753	A	C4-C5-C6	6.07	120.04	117.00
33	BA	1132	A	C4-C5-C6	6.07	120.04	117.00
33	BA	1284	A	N3-C4-N9	6.07	132.26	127.40
33	BA	1672	A	C4-C5-C6	6.07	120.04	117.00
33	BA	1685	A	C4-C5-C6	6.07	120.04	117.00
1	AA	195	A	C4-C5-C6	6.07	120.04	117.00
33	BA	526	A	C4-C5-N7	-6.07	107.66	110.70
33	BA	974	A	N3-C4-N9	6.07	132.26	127.40
33	BA	279	A	C4-C5-C6	6.07	120.03	117.00
33	BA	1174	A	C4-C5-C6	6.07	120.03	117.00
33	BA	1569	A	N3-C4-N9	6.07	132.26	127.40
33	BA	1989	A	C4-C5-C6	6.07	120.04	117.00
33	BA	2066	A	C4-C5-C6	6.07	120.03	117.00
33	BA	2148	A	N3-C4-N9	6.07	132.26	127.40
33	BA	2547	A	N3-C4-N9	6.07	132.26	127.40
33	BA	2827	A	N3-C4-N9	6.07	132.26	127.40
33	BA	2830	A	C4-C5-C6	6.07	120.03	117.00
33	BA	1965	A	C4-C5-C6	6.07	120.03	117.00
1	AA	361	A	N3-C4-N9	6.07	132.25	127.40
33	BA	758	A	C4-C5-C6	6.07	120.03	117.00
33	BA	1424	A	C4-C5-C6	6.07	120.03	117.00
33	BA	2066	A	N3-C4-N9	6.07	132.25	127.40
33	BA	2590	A	C4-C5-C6	6.07	120.03	117.00
33	BA	2924	A	N3-C4-N9	6.07	132.25	127.40
34	BB	71	A	N3-C4-N9	6.07	132.25	127.40
1	AA	696	A	N3-C4-N9	6.07	132.25	127.40
1	AA	1493	A	N3-C4-N9	6.07	132.25	127.40
33	BA	102	A	C4-C5-C6	6.07	120.03	117.00
33	BA	507	A	C4-C5-C6	6.07	120.03	117.00
33	BA	790	A	N3-C4-N9	6.07	132.25	127.40
33	BA	2227	A	N3-C4-N9	6.07	132.25	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	344	A	C4-C5-C6	6.06	120.03	117.00
33	BA	171	A	C4-C5-C6	6.06	120.03	117.00
33	BA	1575	A	N3-C4-N9	6.06	132.25	127.40
33	BA	2461	A	C4-C5-C6	6.06	120.03	117.00
33	BA	2893	A	C8-N9-C4	6.06	108.22	105.80
33	BA	774	A	N3-C4-N9	6.06	132.25	127.40
33	BA	1832	A	C4-C5-C6	6.06	120.03	117.00
33	BA	2381	A	N3-C4-N9	6.06	132.25	127.40
33	BA	538	A	C8-N9-C4	6.06	108.22	105.80
33	BA	958	A	C4-C5-C6	6.06	120.03	117.00
33	BA	1197	A	C4-C5-C6	6.06	120.03	117.00
33	BA	1323	A	C4-C5-C6	6.06	120.03	117.00
33	BA	1615	A	C4-C5-C6	6.06	120.03	117.00
33	BA	1697	A	C4-C5-C6	6.06	120.03	117.00
33	BA	2357	A	C4-C5-C6	6.06	120.03	117.00
1	AA	793	A	N3-C4-N9	6.06	132.25	127.40
33	BA	6	A	N3-C4-N9	6.06	132.25	127.40
33	BA	1074	A	N3-C4-N9	6.06	132.25	127.40
33	BA	1788	A	C4-C5-C6	6.06	120.03	117.00
33	BA	2846	A	N3-C4-N9	6.06	132.24	127.40
1	AA	462	A	N3-C4-N9	6.05	132.24	127.40
1	AA	512	A	C4-C5-C6	6.05	120.03	117.00
33	BA	1606	A	N3-C4-N9	6.05	132.24	127.40
1	AA	1206	A	C4-C5-C6	6.05	120.03	117.00
33	BA	173	A	C4-C5-C6	6.05	120.03	117.00
33	BA	1516	A	C4-C5-C6	6.05	120.03	117.00
1	AA	107	A	C4-C5-C6	6.05	120.03	117.00
1	AA	496	A	N3-C4-N9	6.05	132.24	127.40
1	AA	1435	A	N3-C4-N9	6.05	132.24	127.40
33	BA	230	A	N3-C4-N9	6.05	132.24	127.40
33	BA	318	A	N3-C4-N9	6.05	132.24	127.40
33	BA	876	A	C4-C5-C6	6.05	120.03	117.00
33	BA	925	A	N3-C4-N9	6.05	132.24	127.40
33	BA	1483	A	C4-C5-C6	6.05	120.02	117.00
33	BA	2571	A	C4-C5-C6	6.05	120.03	117.00
33	BA	2845	A	C4-C5-C6	6.05	120.03	117.00
33	BA	2900	A	N3-C4-N9	6.05	132.24	127.40
33	BA	525	A	N3-C4-N9	6.05	132.24	127.40
33	BA	1580	A	C4-C5-C6	6.05	120.02	117.00
33	BA	2228	A	N3-C4-N9	6.05	132.24	127.40
33	BA	1627	A	C4-C5-C6	6.05	120.02	117.00
33	BA	2006	A	C4-C5-C6	6.05	120.02	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	462	A	C4-C5-C6	6.04	120.02	117.00
33	BA	44	A	N3-C4-N9	6.04	132.24	127.40
33	BA	178	A	C4-C5-C6	6.04	120.02	117.00
33	BA	500	A	C4-C5-C6	6.04	120.02	117.00
33	BA	829	A	C4-C5-C6	6.04	120.02	117.00
33	BA	1046	A	N9-C4-C5	6.04	108.22	105.80
33	BA	1680	A	N3-C4-N9	6.04	132.24	127.40
33	BA	1876	A	C4-C5-C6	6.04	120.02	117.00
33	BA	1981	A	C4-C5-C6	6.04	120.02	117.00
1	AA	287	A	C4-C5-C6	6.04	120.02	117.00
1	AA	919	A	C4-C5-C6	6.04	120.02	117.00
33	BA	2100	A	N3-C4-N9	6.04	132.24	127.40
33	BA	2303	A	C4-C5-C6	6.04	120.02	117.00
33	BA	2406	A	C4-C5-C6	6.04	120.02	117.00
1	AA	329	A	C4-C5-C6	6.04	120.02	117.00
1	AA	404	A	N3-C4-N9	6.04	132.23	127.40
1	AA	685	A	C4-C5-C6	6.04	120.02	117.00
1	AA	1014	A	C4-C5-C6	6.04	120.02	117.00
1	AA	1121	A	C4-C5-C6	6.04	120.02	117.00
33	BA	1254	A	C4-C5-C6	6.04	120.02	117.00
33	BA	2047	A	C4-C5-C6	6.04	120.02	117.00
33	BA	2468	A	C4-C5-C6	6.04	120.02	117.00
1	AA	278	A	C4-C5-C6	6.04	120.02	117.00
1	AA	768	A	C4-C5-C6	6.04	120.02	117.00
33	BA	339	A	C4-C5-C6	6.04	120.02	117.00
33	BA	1617	A	C4-C5-C6	6.04	120.02	117.00
1	AA	151	A	N9-C4-C5	6.04	108.22	105.80
1	AA	1270	A	C4-C5-C6	6.04	120.02	117.00
1	AA	1359	A	C4-C5-C6	6.04	120.02	117.00
33	BA	200	A	C4-C5-C6	6.04	120.02	117.00
33	BA	1814	A	N9-C4-C5	6.04	108.22	105.80
33	BA	2364	A	C4-C5-C6	6.04	120.02	117.00
33	BA	2643	A	C4-C5-C6	6.04	120.02	117.00
33	BA	2904	A	C4-C5-C6	6.04	120.02	117.00
1	AA	631	A	N9-C4-C5	6.04	108.22	105.80
1	AA	677	A	C4-C5-C6	6.04	120.02	117.00
1	AA	630	A	N3-C4-N9	6.04	132.23	127.40
1	AA	978	A	C4-C5-C6	6.04	120.02	117.00
33	BA	630	A	N3-C4-N9	6.04	132.23	127.40
33	BA	849	A	C4-C5-C6	6.04	120.02	117.00
33	BA	1685	A	N3-C4-N9	6.04	132.23	127.40
33	BA	2498	A	C4-C5-C6	6.04	120.02	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	314	A	C4-C5-C6	6.03	120.02	117.00
1	AA	475	A	C4-C5-C6	6.03	120.02	117.00
33	BA	769	A	C4-C5-C6	6.03	120.02	117.00
33	BA	1221	A	C4-C5-C6	6.03	120.02	117.00
33	BA	1760	A	C4-C5-C6	6.03	120.02	117.00
33	BA	2734	A	C4-C5-C6	6.03	120.02	117.00
1	AA	459	A	C4-C5-C6	6.03	120.02	117.00
1	AA	1284	A	N3-C4-N9	6.03	132.22	127.40
33	BA	971	A	N3-C4-N9	6.03	132.22	127.40
33	BA	1194	A	C4-C5-C6	6.03	120.02	117.00
33	BA	2091	A	C4-C5-C6	6.03	120.02	117.00
1	AA	81	A	C4-C5-C6	6.03	120.02	117.00
33	BA	2750	A	C8-N9-C4	6.03	108.21	105.80
1	AA	390	A	C4-C5-C6	6.03	120.01	117.00
1	AA	677	A	N3-C4-N9	6.03	132.22	127.40
33	BA	622	A	C4-C5-C6	6.03	120.01	117.00
33	BA	1008	A	N3-C4-N9	6.03	132.22	127.40
33	BA	2700	A	N3-C4-N9	6.03	132.22	127.40
33	BA	2754	A	C4-C5-C6	6.03	120.01	117.00
1	AA	61	A	N3-C4-N9	6.03	132.22	127.40
1	AA	529	A	C4-C5-C6	6.03	120.01	117.00
1	AA	801	A	C4-C5-C6	6.03	120.01	117.00
1	AA	824	A	C4-C5-C6	6.03	120.01	117.00
1	AA	1463	A	N3-C4-N9	6.03	132.22	127.40
33	BA	206	A	C4-C5-C6	6.03	120.01	117.00
33	BA	429	A	N3-C4-N9	6.03	132.22	127.40
33	BA	547	A	C4-C5-C6	6.03	120.01	117.00
33	BA	1284	A	C4-C5-C6	6.03	120.01	117.00
33	BA	2146	A	C4-C5-C6	6.03	120.01	117.00
34	BB	51	A	N3-C4-N9	6.03	132.22	127.40
1	AA	1092	A	C4-C5-C6	6.02	120.01	117.00
1	AA	1366	A	N3-C4-N9	6.02	132.22	127.40
33	BA	179	A	C4-C5-C6	6.02	120.01	117.00
33	BA	281	A	C4-C5-C6	6.02	120.01	117.00
33	BA	329	A	C4-C5-C6	6.02	120.01	117.00
33	BA	330	A	C4-C5-C6	6.02	120.01	117.00
33	BA	652	A	C4-C5-C6	6.02	120.01	117.00
33	BA	894	A	C4-C5-C6	6.02	120.01	117.00
33	BA	1027	A	C4-C5-C6	6.02	120.01	117.00
33	BA	1174	A	N3-C4-N9	6.02	132.22	127.40
33	BA	1388	A	N3-C4-N9	6.02	132.22	127.40
33	BA	1661	A	N9-C4-C5	6.02	108.21	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1054	A	C4-C5-C6	6.02	120.01	117.00
1	AA	1206	A	N3-C4-N9	6.02	132.22	127.40
33	BA	2887	A	N3-C4-N9	6.02	132.22	127.40
1	AA	650	A	N3-C4-N9	6.02	132.22	127.40
1	AA	672	A	C4-C5-C6	6.02	120.01	117.00
1	AA	715	A	N3-C4-N9	6.02	132.22	127.40
1	AA	1261	A	C4-C5-C6	6.02	120.01	117.00
21	AX	44	A	C4-C5-C6	6.02	120.01	117.00
33	BA	231	A	C4-C5-C6	6.02	120.01	117.00
33	BA	1126	A	C4-C5-C6	6.02	120.01	117.00
33	BA	2869	A	C4-C5-C6	6.02	120.01	117.00
1	AA	1022	A	N3-C4-N9	6.02	132.21	127.40
1	AA	1383	A	N3-C4-N9	6.02	132.22	127.40
33	BA	987	A	C4-C5-C6	6.02	120.01	117.00
33	BA	1421	A	N3-C4-N9	6.02	132.21	127.40
33	BA	1608	A	C4-C5-C6	6.02	120.01	117.00
33	BA	1925	A	N3-C4-N9	6.02	132.21	127.40
33	BA	2919	A	N3-C4-N9	6.02	132.21	127.40
1	AA	917	A	N3-C4-N9	6.02	132.21	127.40
33	BA	1406	A	C4-C5-C6	6.02	120.01	117.00
33	BA	2889	A	N3-C4-N9	6.02	132.21	127.40
1	AA	1486	A	N3-C4-N9	6.01	132.21	127.40
33	BA	6	A	C4-C5-C6	6.01	120.01	117.00
33	BA	369	A	N3-C4-N9	6.01	132.21	127.40
33	BA	765	A	N3-C4-N9	6.01	132.21	127.40
33	BA	1585	A	C4-C5-C6	6.01	120.01	117.00
33	BA	2000	A	C4-C5-C6	6.01	120.01	117.00
33	BA	2837	A	C4-C5-C6	6.01	120.01	117.00
1	AA	1128	A	C4-C5-C6	6.01	120.01	117.00
33	BA	236	A	C4-C5-C6	6.01	120.01	117.00
33	BA	1606	A	C4-C5-C6	6.01	120.01	117.00
33	BA	2830	A	N3-C4-N9	6.01	132.21	127.40
1	AA	1348	A	N3-C4-N9	6.01	132.21	127.40
33	BA	705	A	C4-C5-C6	6.01	120.00	117.00
33	BA	1895	A	N3-C4-N9	6.01	132.21	127.40
33	BA	2047	A	N3-C4-N9	6.01	132.21	127.40
33	BA	2356	A	C4-C5-C6	6.01	120.00	117.00
33	BA	486	A	C4-C5-C6	6.01	120.00	117.00
33	BA	753	A	N3-C4-N9	6.01	132.21	127.40
33	BA	993	A	C4-C5-C6	6.01	120.00	117.00
33	BA	2089	A	C8-N9-C4	6.01	108.20	105.80
1	AA	381	A	C4-C5-C6	6.01	120.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1532	A	C4-C5-C6	6.01	120.00	117.00
33	BA	2389	A	C4-C5-C6	6.01	120.00	117.00
1	AA	650	A	C4-C5-C6	6.01	120.00	117.00
1	AA	1333	A	C4-C5-C6	6.01	120.00	117.00
33	BA	449	A	C4-C5-C6	6.01	120.00	117.00
33	BA	1235	A	N3-C4-N9	6.01	132.21	127.40
33	BA	2421	A	C4-C5-C6	6.01	120.00	117.00
33	BA	2769	A	C4-C5-C6	6.01	120.00	117.00
1	AA	271	A	C4-C5-C6	6.00	120.00	117.00
33	BA	978	A	C4-C5-C6	6.00	120.00	117.00
33	BA	1453	A	C4-C5-C6	6.00	120.00	117.00
33	BA	2661	A	C4-C5-C6	6.00	120.00	117.00
34	BB	114	A	C4-C5-C6	6.00	120.00	117.00
1	AA	604	A	C4-C5-C6	6.00	120.00	117.00
1	AA	862	A	C4-C5-N7	-6.00	107.70	110.70
1	AA	1188	A	N3-C4-N9	6.00	132.20	127.40
33	BA	278	A	C4-C5-C6	6.00	120.00	117.00
33	BA	1113	A	C4-C5-C6	6.00	120.00	117.00
33	BA	1201	A	N9-C4-C5	6.00	108.20	105.80
33	BA	1423	A	C4-C5-C6	6.00	120.00	117.00
33	BA	2454	A	N3-C4-N9	6.00	132.20	127.40
34	BB	55	A	C4-C5-C6	6.00	120.00	117.00
1	AA	270	A	N3-C4-N9	6.00	132.20	127.40
1	AA	929	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1513	A	C4-C5-C6	6.00	120.00	117.00
33	BA	500	A	N3-C4-N9	6.00	132.20	127.40
33	BA	763	A	C4-C5-C6	6.00	120.00	117.00
33	BA	1197	A	N3-C4-N9	6.00	132.20	127.40
33	BA	1461	A	N3-C4-N9	6.00	132.20	127.40
34	BB	43	A	C4-C5-C6	6.00	120.00	117.00
1	AA	381	A	N3-C4-N9	6.00	132.20	127.40
1	AA	1161	A	N3-C4-N9	6.00	132.20	127.40
1	AA	35	A	C4-C5-C6	6.00	120.00	117.00
1	AA	139	A	C4-C5-C6	6.00	120.00	117.00
1	AA	234	A	N3-C4-N9	6.00	132.20	127.40
1	AA	928	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1245	A	C4-C5-C6	6.00	120.00	117.00
33	BA	574	A	C4-C5-C6	6.00	120.00	117.00
33	BA	1260	A	C4-C5-C6	6.00	120.00	117.00
33	BA	1789	A	C4-C5-C6	6.00	120.00	117.00
33	BA	2032	A	C4-C5-C6	6.00	120.00	117.00
33	BA	2216	A	C4-C5-C6	6.00	120.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	173	A	N3-C4-N9	6.00	132.20	127.40
1	AA	190	A	C4-C5-C6	6.00	120.00	117.00
1	AA	874	A	N3-C4-N9	6.00	132.20	127.40
1	AA	1180	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1327	A	N3-C4-N9	6.00	132.20	127.40
1	AA	1425	A	N3-C4-N9	6.00	132.20	127.40
33	BA	1055	A	C4-C5-C6	6.00	120.00	117.00
33	BA	1130	A	C4-C5-C6	6.00	120.00	117.00
33	BA	1230	A	C4-C5-C6	6.00	120.00	117.00
33	BA	1556	A	N3-C4-N9	6.00	132.20	127.40
33	BA	2365	A	C8-N9-C4	6.00	108.20	105.80
33	BA	2668	A	C4-C5-C6	6.00	120.00	117.00
33	BA	1608	A	N3-C4-N9	6.00	132.20	127.40
33	BA	2787	A	C4-C5-C6	6.00	120.00	117.00
33	BA	2902	A	C4-C5-C6	6.00	120.00	117.00
1	AA	532	A	C4-C5-C6	5.99	120.00	117.00
1	AA	659	A	C4-C5-C6	5.99	120.00	117.00
1	AA	979	A	C4-C5-C6	5.99	120.00	117.00
33	BA	436	A	C4-C5-C6	5.99	120.00	117.00
33	BA	922	A	C4-C5-C6	5.99	120.00	117.00
33	BA	1025	A	C4-C5-C6	5.99	120.00	117.00
33	BA	1615	A	N3-C4-N9	5.99	132.19	127.40
33	BA	2049	A	N3-C4-N9	5.99	132.19	127.40
33	BA	2256	A	C4-C5-C6	5.99	120.00	117.00
33	BA	2619	A	N3-C4-N9	5.99	132.19	127.40
1	AA	504	A	C4-C5-C6	5.99	120.00	117.00
33	BA	260	A	N3-C4-N9	5.99	132.19	127.40
1	AA	968	A	C4-C5-C6	5.99	120.00	117.00
1	AA	1523	A	C4-C5-C6	5.99	120.00	117.00
33	BA	259	A	N3-C4-N9	5.99	132.19	127.40
33	BA	1404	A	C4-C5-C6	5.99	120.00	117.00
33	BA	1631	A	C4-C5-C6	5.99	120.00	117.00
33	BA	124	A	C4-C5-C6	5.99	119.99	117.00
33	BA	268	A	C4-C5-C6	5.99	119.99	117.00
33	BA	2629	A	N3-C4-N9	5.99	132.19	127.40
33	BA	2834	A	C4-C5-C6	5.99	119.99	117.00
33	BA	324	A	C8-N9-C4	5.99	108.19	105.80
33	BA	2298	A	C4-C5-C6	5.99	119.99	117.00
33	BA	2477	A	C4-C5-C6	5.99	119.99	117.00
1	AA	117	A	C4-C5-C6	5.99	119.99	117.00
1	AA	382	A	N3-C4-N9	5.99	132.19	127.40
21	AX	41	A	N3-C4-N9	5.99	132.19	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	623	A	N3-C4-N9	5.99	132.19	127.40
33	BA	952	A	C4-C5-C6	5.99	119.99	117.00
33	BA	1404	A	N3-C4-N9	5.99	132.19	127.40
33	BA	1417	A	N9-C4-C5	5.99	108.19	105.80
33	BA	1464	A	C4-C5-C6	5.99	119.99	117.00
34	BB	64	A	N3-C4-N9	5.99	132.19	127.40
1	AA	618	A	C4-C5-C6	5.98	119.99	117.00
33	BA	384	A	C4-C5-C6	5.98	119.99	117.00
33	BA	1005	A	N3-C4-N9	5.98	132.19	127.40
33	BA	1260	A	N3-C4-N9	5.98	132.19	127.40
33	BA	2119	A	C4-C5-C6	5.98	119.99	117.00
33	BA	2468	A	N3-C4-N9	5.98	132.19	127.40
33	BA	2511	A	N3-C4-N9	5.98	132.19	127.40
33	BA	2719	A	N3-C4-N9	5.98	132.19	127.40
1	AA	364	A	N3-C4-N9	5.98	132.19	127.40
1	AA	870	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1320	A	C4-C5-C6	5.98	119.99	117.00
33	BA	1312	A	C4-C5-C6	5.98	119.99	117.00
33	BA	1723	A	C4-C5-C6	5.98	119.99	117.00
33	BA	2658	A	C4-C5-C6	5.98	119.99	117.00
1	AA	371	A	C4-C5-C6	5.98	119.99	117.00
1	AA	669	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1077	A	C8-N9-C4	5.98	108.19	105.80
33	BA	376	A	N3-C4-N9	5.98	132.19	127.40
33	BA	1918	A	C4-C5-C6	5.98	119.99	117.00
33	BA	2220	A	N3-C4-N9	5.98	132.18	127.40
33	BA	2770	A	C4-C5-C6	5.98	119.99	117.00
1	AA	53	A	C4-C5-C6	5.98	119.99	117.00
1	AA	725	A	C4-C5-C6	5.98	119.99	117.00
33	BA	786	A	C4-C5-C6	5.98	119.99	117.00
33	BA	2734	A	N3-C4-N9	5.98	132.18	127.40
34	BB	64	A	C4-C5-C6	5.98	119.99	117.00
1	AA	796	A	C4-C5-C6	5.98	119.99	117.00
33	BA	459	A	N3-C4-N9	5.98	132.18	127.40
33	BA	469	A	N3-C4-N9	5.98	132.18	127.40
33	BA	519	A	C4-C5-C6	5.98	119.99	117.00
33	BA	1027	A	N3-C4-N9	5.98	132.18	127.40
33	BA	1542	A	C4-C5-C6	5.98	119.99	117.00
33	BA	1583	A	N3-C4-N9	5.98	132.18	127.40
33	BA	1663	A	C4-C5-C6	5.98	119.99	117.00
33	BA	1743	A	C4-C5-C6	5.98	119.99	117.00
33	BA	1774	A	N3-C4-N9	5.98	132.18	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2018	A	C4-C5-C6	5.98	119.99	117.00
33	BA	2316	A	N3-C4-N9	5.98	132.18	127.40
1	AA	684	A	C4-C5-C6	5.98	119.99	117.00
1	AA	985	A	C8-N9-C4	5.98	108.19	105.80
33	BA	1592	A	C4-C5-C6	5.98	119.99	117.00
33	BA	1735	A	C4-C5-C6	5.98	119.99	117.00
33	BA	2594	A	C4-C5-C6	5.98	119.99	117.00
33	BA	2708	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1022	A	C4-C5-C6	5.97	119.99	117.00
33	BA	479	A	C4-C5-C6	5.97	119.99	117.00
33	BA	543	A	C4-C5-C6	5.97	119.99	117.00
33	BA	830	A	C4-C5-C6	5.97	119.99	117.00
33	BA	908	A	C4-C5-C6	5.97	119.99	117.00
33	BA	1636	A	N3-C4-N9	5.97	132.18	127.40
33	BA	2498	A	N3-C4-N9	5.97	132.18	127.40
1	AA	519	A	C4-C5-C6	5.97	119.99	117.00
1	AA	1222	A	N3-C4-N9	5.97	132.18	127.40
33	BA	507	A	N3-C4-N9	5.97	132.18	127.40
33	BA	658	A	C4-C5-C6	5.97	119.99	117.00
33	BA	904	A	C4-C5-C6	5.97	119.99	117.00
33	BA	1760	A	N3-C4-N9	5.97	132.18	127.40
33	BA	1942	A	C4-C5-C6	5.97	119.99	117.00
33	BA	2087	A	C4-C5-C6	5.97	119.99	117.00
33	BA	2124	A	N3-C4-N9	5.97	132.18	127.40
33	BA	2124	A	C4-C5-C6	5.97	119.99	117.00
33	BA	2616	A	N3-C4-N9	5.97	132.18	127.40
1	AA	886	A	C4-C5-C6	5.97	119.98	117.00
33	BA	537	A	N3-C4-N9	5.97	132.18	127.40
33	BA	868	A	N3-C4-N9	5.97	132.18	127.40
33	BA	1029	A	C4-C5-C6	5.97	119.99	117.00
33	BA	2819	A	C8-N9-C4	5.97	108.19	105.80
33	BA	2854	A	N3-C4-N9	5.97	132.18	127.40
1	AA	210	A	C4-C5-C6	5.97	119.98	117.00
1	AA	1028	A	C4-C5-C6	5.97	119.98	117.00
1	AA	1103	A	C4-C5-C6	5.97	119.98	117.00
1	AA	1407	A	C8-N9-C4	5.97	108.19	105.80
1	AA	1509	A	C4-C5-C6	5.97	119.98	117.00
33	BA	561	A	C4-C5-C6	5.97	119.98	117.00
33	BA	722	A	C8-N9-C4	5.97	108.19	105.80
33	BA	1361	A	C4-C5-C6	5.97	119.98	117.00
33	BA	1534	A	C4-C5-C6	5.97	119.98	117.00
33	BA	1583	A	C4-C5-C6	5.97	119.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1648	A	C4-C5-C6	5.97	119.98	117.00
33	BA	1818	A	C4-C5-C6	5.97	119.98	117.00
33	BA	2338	A	C4-C5-C6	5.97	119.98	117.00
1	AA	724	A	C4-C5-C6	5.97	119.98	117.00
1	AA	879	A	C8-N9-C4	5.97	108.19	105.80
1	AA	902	A	N3-C4-N9	5.97	132.18	127.40
33	BA	2462	A	C4-C5-C6	5.97	119.98	117.00
33	BA	2875	A	C4-C5-C6	5.97	119.98	117.00
1	AA	415	A	C8-N9-C4	5.97	108.19	105.80
1	AA	703	A	C8-N9-C4	5.97	108.19	105.80
33	BA	428	A	C4-C5-C6	5.97	119.98	117.00
33	BA	925	A	C4-C5-C6	5.97	119.98	117.00
1	AA	1147	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1479	A	C4-C5-C6	5.96	119.98	117.00
21	AX	76	A	N3-C4-N9	5.96	132.17	127.40
33	BA	13	A	C4-C5-C6	5.96	119.98	117.00
33	BA	808	A	C4-C5-C6	5.96	119.98	117.00
33	BA	893	A	C4-C5-C6	5.96	119.98	117.00
33	BA	1424	A	C8-N9-C4	5.96	108.19	105.80
33	BA	1617	A	N3-C4-N9	5.96	132.17	127.40
33	BA	2593	A	C4-C5-C6	5.96	119.98	117.00
34	BB	20	A	N3-C4-N9	5.96	132.17	127.40
1	AA	81	A	N3-C4-N9	5.96	132.17	127.40
33	BA	1131	A	N3-C4-N9	5.96	132.17	127.40
33	BA	2750	A	C4-C5-C6	5.96	119.98	117.00
34	BB	18	A	C4-C5-C6	5.96	119.98	117.00
33	BA	705	A	N3-C4-N9	5.96	132.17	127.40
33	BA	1042	A	C4-C5-C6	5.96	119.98	117.00
33	BA	1848	A	N3-C4-N9	5.96	132.17	127.40
33	BA	2417	A	C4-C5-C6	5.96	119.98	117.00
34	BB	71	A	C4-C5-C6	5.96	119.98	117.00
1	AA	522	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1529	A	C4-C5-C6	5.96	119.98	117.00
33	BA	2062	A	N9-C4-C5	5.96	108.18	105.80
1	AA	1247	A	N9-C4-C5	5.96	108.18	105.80
1	AA	1270	A	N3-C4-N9	5.96	132.17	127.40
33	BA	10	A	C4-C5-C6	5.96	119.98	117.00
33	BA	758	A	N3-C4-N9	5.96	132.17	127.40
33	BA	1405	A	C4-C5-C6	5.96	119.98	117.00
33	BA	1774	A	C4-C5-C6	5.96	119.98	117.00
33	BA	1838	A	C4-C5-C6	5.96	119.98	117.00
33	BA	2851	A	N3-C4-N9	5.96	132.17	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	281	A	C4-C5-C6	5.96	119.98	117.00
1	AA	364	A	C4-C5-C6	5.96	119.98	117.00
1	AA	650	A	C8-N9-C4	5.96	108.18	105.80
1	AA	1328	A	C4-C5-C6	5.96	119.98	117.00
33	BA	1026	A	C4-C5-C6	5.96	119.98	117.00
33	BA	2526	A	C4-C5-C6	5.96	119.98	117.00
33	BA	2782	A	C4-C5-C6	5.96	119.98	117.00
34	BB	50	A	N3-C4-N9	5.96	132.17	127.40
1	AA	705	A	N3-C4-N9	5.96	132.16	127.40
33	BA	957	A	C4-C5-C6	5.96	119.98	117.00
33	BA	1003	A	C8-N9-C4	5.96	108.18	105.80
33	BA	1947	A	N3-C4-N9	5.96	132.16	127.40
33	BA	2770	A	C8-N9-C4	5.96	108.18	105.80
33	BA	2907	A	C4-C5-C6	5.96	119.98	117.00
1	AA	296	A	C4-C5-C6	5.95	119.98	117.00
1	AA	604	A	N3-C4-N9	5.95	132.16	127.40
33	BA	307	A	C4-C5-C6	5.95	119.98	117.00
33	BA	1593	A	C4-C5-C6	5.95	119.98	117.00
33	BA	1956	A	N3-C4-N9	5.95	132.16	127.40
33	BA	2750	A	N3-C4-N9	5.95	132.16	127.40
33	BA	2778	A	C4-C5-C6	5.95	119.98	117.00
33	BA	2889	A	C4-C5-C6	5.95	119.98	117.00
1	AA	344	A	N3-C4-N9	5.95	132.16	127.40
1	AA	947	A	C4-C5-C6	5.95	119.98	117.00
1	AA	1031	A	C4-C5-C6	5.95	119.98	117.00
33	BA	330	A	N3-C4-N9	5.95	132.16	127.40
33	BA	2060	A	C4-C5-C6	5.95	119.98	117.00
33	BA	2887	A	C4-C5-C6	5.95	119.98	117.00
1	AA	357	A	C4-C5-C6	5.95	119.97	117.00
1	AA	1024	A	N3-C4-N9	5.95	132.16	127.40
33	BA	194	A	N3-C4-N9	5.95	132.16	127.40
33	BA	560	A	C4-C5-C6	5.95	119.97	117.00
33	BA	1291	A	C4-C5-C6	5.95	119.98	117.00
33	BA	1308	A	C8-N9-C4	5.95	108.18	105.80
33	BA	1555	A	N9-C4-C5	5.95	108.18	105.80
33	BA	1675	A	N3-C4-N9	5.95	132.16	127.40
33	BA	1700	A	C8-N9-C4	5.95	108.18	105.80
1	AA	61	A	C4-C5-C6	5.95	119.97	117.00
1	AA	382	A	C4-C5-C6	5.95	119.97	117.00
1	AA	452	A	C4-C5-C6	5.95	119.97	117.00
1	AA	672	A	N3-C4-N9	5.95	132.16	127.40
1	AA	1294	A	N3-C4-N9	5.95	132.16	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	769	A	N3-C4-N9	5.95	132.16	127.40
33	BA	1021	A	C4-C5-C6	5.95	119.97	117.00
33	BA	1131	A	C4-C5-C6	5.95	119.97	117.00
33	BA	1233	A	N3-C4-N9	5.95	132.16	127.40
33	BA	2505	A	N3-C4-N9	5.95	132.16	127.40
33	BA	2787	A	N3-C4-N9	5.95	132.16	127.40
33	BA	1265	A	N3-C4-N9	5.95	132.16	127.40
1	AA	117	A	N3-C4-N9	5.95	132.16	127.40
1	AA	150	A	N9-C4-C5	5.95	108.18	105.80
1	AA	555	A	N9-C4-C5	5.95	108.18	105.80
1	AA	824	A	N3-C4-N9	5.95	132.16	127.40
1	AA	1528	A	C4-C5-C6	5.95	119.97	117.00
33	BA	102	A	N3-C4-N9	5.95	132.16	127.40
33	BA	307	A	N3-C4-N9	5.95	132.16	127.40
33	BA	821	A	C8-N9-C4	5.95	108.18	105.80
33	BA	847	A	C8-N9-C4	5.95	108.18	105.80
33	BA	1928	A	C4-C5-C6	5.95	119.97	117.00
33	BA	2440	A	C4-C5-C6	5.95	119.97	117.00
33	BA	2804	A	C4-C5-C6	5.95	119.97	117.00
34	BB	51	A	C4-C5-C6	5.95	119.97	117.00
1	AA	94	A	N3-C4-N9	5.94	132.16	127.40
1	AA	1455	A	N3-C4-N9	5.94	132.16	127.40
33	BA	337	A	C4-C5-C6	5.94	119.97	117.00
33	BA	1054	A	N3-C4-N9	5.94	132.16	127.40
33	BA	1813	A	C4-C5-C6	5.94	119.97	117.00
34	BB	56	A	C4-C5-C6	5.94	119.97	117.00
1	AA	10	A	C8-N9-C4	5.94	108.18	105.80
1	AA	251	A	C4-C5-C6	5.94	119.97	117.00
1	AA	1092	A	N3-C4-N9	5.94	132.15	127.40
1	AA	1178	A	C4-C5-C6	5.94	119.97	117.00
1	AA	1455	A	C4-C5-C6	5.94	119.97	117.00
33	BA	584	A	C8-N9-C4	5.94	108.18	105.80
33	BA	678	A	N3-C4-N9	5.94	132.15	127.40
33	BA	1277	A	C4-C5-C6	5.94	119.97	117.00
33	BA	2042	A	N3-C4-N9	5.94	132.15	127.40
33	BA	2165	A	C4-C5-C6	5.94	119.97	117.00
33	BA	2307	A	C4-C5-C6	5.94	119.97	117.00
33	BA	2462	A	N3-C4-N9	5.94	132.16	127.40
1	AA	796	A	N3-C4-N9	5.94	132.15	127.40
33	BA	388	A	C4-C5-C6	5.94	119.97	117.00
33	BA	637	A	C4-C5-C6	5.94	119.97	117.00
33	BA	1445	A	N3-C4-N9	5.94	132.15	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1585	A	N3-C4-N9	5.94	132.15	127.40
33	BA	1627	A	N3-C4-N9	5.94	132.15	127.40
33	BA	1925	A	C4-C5-C6	5.94	119.97	117.00
33	BA	2505	A	C4-C5-C6	5.94	119.97	117.00
1	AA	352	A	C4-C5-C6	5.94	119.97	117.00
1	AA	786	A	C4-C5-C6	5.94	119.97	117.00
1	AA	1257	A	C4-C5-C6	5.94	119.97	117.00
33	BA	14	A	C4-C5-C6	5.94	119.97	117.00
1	AA	34	A	N3-C4-N9	5.94	132.15	127.40
1	AA	323	A	C4-C5-C6	5.94	119.97	117.00
1	AA	771	A	C4-C5-C6	5.94	119.97	117.00
1	AA	1260	A	N3-C4-N9	5.94	132.15	127.40
1	AA	1296	A	N3-C4-N9	5.94	132.15	127.40
1	AA	1403	A	C4-C5-C6	5.94	119.97	117.00
33	BA	110	A	C4-C5-C6	5.94	119.97	117.00
33	BA	600	A	C4-C5-C6	5.94	119.97	117.00
33	BA	781	A	C4-C5-C6	5.94	119.97	117.00
33	BA	1233	A	C4-C5-C6	5.94	119.97	117.00
33	BA	1721	A	N3-C4-N9	5.94	132.15	127.40
33	BA	2463	A	C4-C5-C6	5.94	119.97	117.00
1	AA	491	A	C4-C5-C6	5.94	119.97	117.00
33	BA	373	A	C4-C5-C6	5.94	119.97	117.00
33	BA	702	A	C8-N9-C4	5.94	108.17	105.80
33	BA	957	A	N3-C4-N9	5.94	132.15	127.40
33	BA	2187	A	C8-N9-C4	5.94	108.17	105.80
33	BA	2317	A	C4-C5-C6	5.94	119.97	117.00
33	BA	2461	A	N3-C4-N9	5.94	132.15	127.40
1	AA	314	A	N3-C4-N9	5.93	132.15	127.40
1	AA	1014	A	N3-C4-N9	5.93	132.15	127.40
1	AA	1296	A	C4-C5-C6	5.93	119.97	117.00
1	AA	1359	A	N3-C4-N9	5.93	132.15	127.40
21	AX	23	A	N3-C4-N9	5.93	132.15	127.40
33	BA	67	A	C4-C5-C6	5.93	119.97	117.00
33	BA	762	A	C4-C5-C6	5.93	119.97	117.00
33	BA	1144	A	C4-C5-C6	5.93	119.97	117.00
33	BA	1483	A	N3-C4-N9	5.93	132.15	127.40
33	BA	1541	A	N3-C4-N9	5.93	132.15	127.40
1	AA	1065	A	C8-N9-C4	5.93	108.17	105.80
1	AA	1115	A	C4-C5-C6	5.93	119.97	117.00
1	AA	1176	A	C4-C5-C6	5.93	119.97	117.00
21	AX	58	A	N3-C4-N9	5.93	132.15	127.40
33	BA	275	A	N3-C4-N9	5.93	132.15	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	333	A	C4-C5-C6	5.93	119.97	117.00
33	BA	384	A	N3-C4-N9	5.93	132.15	127.40
33	BA	1066	A	C4-C5-C6	5.93	119.97	117.00
33	BA	1473	A	C8-N9-C4	5.93	108.17	105.80
33	BA	1532	A	N3-C4-N9	5.93	132.15	127.40
33	BA	1588	A	C4-C5-C6	5.93	119.97	117.00
34	BB	76	A	C4-C5-C6	5.93	119.97	117.00
1	AA	1502	A	C4-C5-C6	5.93	119.97	117.00
33	BA	64	A	C8-N9-C4	5.93	108.17	105.80
33	BA	150	A	C4-C5-C6	5.93	119.97	117.00
33	BA	279	A	N3-C4-N9	5.93	132.15	127.40
33	BA	1326	A	C4-C5-C6	5.93	119.97	117.00
33	BA	1520	A	C4-C5-C6	5.93	119.97	117.00
33	BA	1850	A	C4-C5-C6	5.93	119.97	117.00
33	BA	2330	A	C4-C5-C6	5.93	119.97	117.00
33	BA	548	A	C4-C5-C6	5.93	119.96	117.00
33	BA	867	A	C4-C5-C6	5.93	119.97	117.00
33	BA	1034	A	C8-N9-C4	5.93	108.17	105.80
33	BA	1042	A	N3-C4-N9	5.93	132.14	127.40
33	BA	1456	A	C4-C5-C6	5.93	119.97	117.00
33	BA	1791	A	C4-C5-C6	5.93	119.97	117.00
1	AA	638	A	C4-C5-C6	5.93	119.96	117.00
1	AA	664	A	C4-C5-C6	5.93	119.96	117.00
33	BA	222	A	C4-C5-C6	5.93	119.96	117.00
33	BA	421	A	C4-C5-C6	5.93	119.96	117.00
33	BA	2542	A	C4-C5-C6	5.93	119.96	117.00
33	BA	2590	A	N3-C4-N9	5.93	132.14	127.40
1	AA	204	A	C4-C5-C6	5.93	119.96	117.00
21	AX	41	A	C4-C5-C6	5.93	119.96	117.00
33	BA	94	A	C4-C5-C6	5.93	119.96	117.00
33	BA	993	A	N3-C4-N9	5.93	132.14	127.40
33	BA	1188	A	N9-C4-C5	5.93	108.17	105.80
33	BA	1767	A	N3-C4-N9	5.93	132.14	127.40
33	BA	2078	A	N3-C4-N9	5.93	132.14	127.40
1	AA	67	A	C4-C5-C6	5.92	119.96	117.00
1	AA	583	A	C4-C5-C6	5.92	119.96	117.00
1	AA	790	A	C8-N9-C4	5.92	108.17	105.80
1	AA	1213	A	N9-C4-C5	5.92	108.17	105.80
1	AA	1260	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1271	A	C4-C5-C6	5.92	119.96	117.00
33	BA	12	A	N3-C4-N9	5.92	132.14	127.40
33	BA	582	A	C4-C5-C6	5.92	119.96	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	740	A	C4-C5-C6	5.92	119.96	117.00
33	BA	770	A	C4-C5-C6	5.92	119.96	117.00
33	BA	947	A	N3-C4-N9	5.92	132.14	127.40
33	BA	1014	A	C4-C5-C6	5.92	119.96	117.00
33	BA	1116	A	C4-C5-C6	5.92	119.96	117.00
33	BA	1434	A	N9-C4-C5	5.92	108.17	105.80
33	BA	1648	A	N3-C4-N9	5.92	132.14	127.40
33	BA	1663	A	N3-C4-N9	5.92	132.14	127.40
33	BA	2389	A	N3-C4-N9	5.92	132.14	127.40
33	BA	2497	A	N3-C4-N9	5.92	132.14	127.40
33	BA	2601	A	C8-N9-C4	5.92	108.17	105.80
1	AA	658	A	C4-C5-C6	5.92	119.96	117.00
1	AA	874	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1178	A	N3-C4-N9	5.92	132.14	127.40
33	BA	1047	A	N3-C4-N9	5.92	132.14	127.40
33	BA	1588	A	N3-C4-N9	5.92	132.14	127.40
33	BA	2719	A	C4-C5-C6	5.92	119.96	117.00
34	BB	25	A	N3-C4-N9	5.92	132.14	127.40
34	BB	44	A	C4-C5-C6	5.92	119.96	117.00
1	AA	35	A	N3-C4-N9	5.92	132.14	127.40
1	AA	160	A	C4-C5-C6	5.92	119.96	117.00
1	AA	240	A	C4-C5-C6	5.92	119.96	117.00
1	AA	463	A	C4-C5-C6	5.92	119.96	117.00
1	AA	644	A	N3-C4-N9	5.92	132.14	127.40
1	AA	737	A	N9-C4-C5	5.92	108.17	105.80
21	AX	14	A	N3-C4-N9	5.92	132.14	127.40
21	AX	21	A	N3-C4-N9	5.92	132.14	127.40
33	BA	324	A	N3-C4-N9	5.92	132.14	127.40
33	BA	337	A	N3-C4-N9	5.92	132.14	127.40
33	BA	438	A	C4-C5-C6	5.92	119.96	117.00
33	BA	449	A	N3-C4-N9	5.92	132.14	127.40
33	BA	659	A	C4-C5-C6	5.92	119.96	117.00
33	BA	762	A	N3-C4-N9	5.92	132.14	127.40
33	BA	888	A	C4-C5-C6	5.92	119.96	117.00
33	BA	1734	A	C4-C5-C6	5.92	119.96	117.00
33	BA	1815	A	C8-N9-C4	5.92	108.17	105.80
33	BA	1945	A	N3-C4-N9	5.92	132.14	127.40
33	BA	2383	A	C4-C5-C6	5.92	119.96	117.00
33	BA	2482	A	C4-C5-C6	5.92	119.96	117.00
33	BA	2876	A	C4-C5-C6	5.92	119.96	117.00
33	BA	71	A	N3-C4-N9	5.92	132.14	127.40
33	BA	1499	A	C4-C5-C6	5.92	119.96	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2026	A	C8-N9-C4	5.92	108.17	105.80
33	BA	2893	A	N3-C4-N9	5.92	132.14	127.40
1	AA	203	A	C4-C5-C6	5.92	119.96	117.00
1	AA	390	A	N3-C4-N9	5.92	132.13	127.40
1	AA	460	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1252	A	N3-C4-N9	5.92	132.13	127.40
33	BA	355	A	C4-C5-C6	5.92	119.96	117.00
33	BA	364	A	C4-C5-C6	5.92	119.96	117.00
33	BA	412	A	N3-C4-N9	5.92	132.13	127.40
33	BA	524	A	N3-C4-N9	5.92	132.13	127.40
33	BA	1179	A	C4-C5-C6	5.92	119.96	117.00
33	BA	1555	A	C4-C5-N7	-5.92	107.74	110.70
33	BA	1961	A	N3-C4-N9	5.92	132.13	127.40
33	BA	2570	A	N3-C4-N9	5.92	132.13	127.40
1	AA	62	A	C4-C5-C6	5.92	119.96	117.00
1	AA	529	A	N3-C4-N9	5.92	132.13	127.40
1	AA	658	A	N3-C4-N9	5.92	132.13	127.40
1	AA	831	A	C4-C5-C6	5.92	119.96	117.00
33	BA	198	A	C4-C5-C6	5.92	119.96	117.00
33	BA	207	A	C8-N9-C4	5.92	108.17	105.80
33	BA	388	A	N3-C4-N9	5.92	132.13	127.40
33	BA	1813	A	N3-C4-N9	5.92	132.13	127.40
33	BA	2119	A	N3-C4-N9	5.92	132.13	127.40
33	BA	2704	A	N3-C4-N9	5.92	132.13	127.40
1	AA	592	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1509	A	N3-C4-N9	5.92	132.13	127.40
33	BA	305	A	C4-C5-C6	5.92	119.96	117.00
33	BA	1059	A	N3-C4-N9	5.92	132.13	127.40
1	AA	52	A	N3-C4-N9	5.91	132.13	127.40
1	AA	791	A	C4-C5-C6	5.91	119.96	117.00
1	AA	825	A	C4-C5-C6	5.91	119.96	117.00
1	AA	1213	A	C4-C5-N7	-5.91	107.74	110.70
1	AA	1266	A	C4-C5-C6	5.91	119.96	117.00
33	BA	216	A	N3-C4-N9	5.91	132.13	127.40
33	BA	412	A	C4-C5-C6	5.91	119.96	117.00
33	BA	1078	A	N9-C4-C5	5.91	108.17	105.80
33	BA	1094	A	C8-N9-C4	5.91	108.17	105.80
33	BA	1928	A	N3-C4-N9	5.91	132.13	127.40
33	BA	13	A	N3-C4-N9	5.91	132.13	127.40
33	BA	140	A	N3-C4-N9	5.91	132.13	127.40
33	BA	1882	A	N3-C4-N9	5.91	132.13	127.40
33	BA	1919	A	N9-C4-C5	5.91	108.17	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	118	A	C4-C5-C6	5.91	119.95	117.00
1	AA	644	A	C4-C5-C6	5.91	119.96	117.00
1	AA	679	A	N3-C4-N9	5.91	132.13	127.40
1	AA	771	A	N3-C4-N9	5.91	132.13	127.40
1	AA	1259	A	C4-C5-C6	5.91	119.96	117.00
1	AA	1327	A	C4-C5-C6	5.91	119.95	117.00
21	AX	44	A	N3-C4-N9	5.91	132.13	127.40
33	BA	173	A	N3-C4-N9	5.91	132.13	127.40
33	BA	329	A	N3-C4-N9	5.91	132.13	127.40
33	BA	524	A	C4-C5-C6	5.91	119.96	117.00
33	BA	808	A	N3-C4-N9	5.91	132.13	127.40
33	BA	1313	A	C4-C5-C6	5.91	119.95	117.00
33	BA	1375	A	N3-C4-N9	5.91	132.13	127.40
33	BA	1802	A	C4-C5-C6	5.91	119.95	117.00
33	BA	1941	A	N9-C4-C5	5.91	108.16	105.80
33	BA	2340	A	C4-C5-C6	5.91	119.95	117.00
33	BA	2708	A	C8-N9-C4	5.91	108.16	105.80
1	AA	474	A	C4-C5-C6	5.91	119.95	117.00
1	AA	611	A	N3-C4-N9	5.91	132.13	127.40
1	AA	616	A	C4-C5-C6	5.91	119.95	117.00
1	AA	799	A	C4-C5-C6	5.91	119.95	117.00
33	BA	65	A	C4-C5-C6	5.91	119.95	117.00
33	BA	200	A	N3-C4-N9	5.91	132.13	127.40
33	BA	202	A	C4-C5-C6	5.91	119.95	117.00
33	BA	369	A	C4-C5-C6	5.91	119.95	117.00
33	BA	667	A	C4-C5-C6	5.91	119.95	117.00
33	BA	1074	A	C4-C5-C6	5.91	119.95	117.00
33	BA	1266	A	C4-C5-C6	5.91	119.95	117.00
33	BA	2165	A	N3-C4-N9	5.91	132.13	127.40
33	BA	2740	A	C4-C5-C6	5.91	119.95	117.00
1	AA	1248	A	C4-C5-C6	5.91	119.95	117.00
1	AA	1283	A	N3-C4-N9	5.91	132.12	127.40
33	BA	5	A	C4-C5-C6	5.91	119.95	117.00
33	BA	2668	A	N3-C4-N9	5.91	132.12	127.40
1	AA	12	A	C4-C5-C6	5.91	119.95	117.00
1	AA	118	A	N3-C4-N9	5.91	132.12	127.40
1	AA	500	A	C4-C5-N7	-5.91	107.75	110.70
1	AA	762	A	C4-C5-C6	5.91	119.95	117.00
1	AA	816	A	C4-C5-C6	5.91	119.95	117.00
33	BA	206	A	N3-C4-N9	5.91	132.12	127.40
33	BA	1361	A	N3-C4-N9	5.91	132.12	127.40
33	BA	1398	A	C5-C6-N1	5.91	120.65	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1905	A	N9-C4-C5	5.91	108.16	105.80
33	BA	2477	A	N3-C4-N9	5.91	132.12	127.40
33	BA	2807	A	C8-N9-C4	5.91	108.16	105.80
1	AA	506	A	C4-C5-C6	5.90	119.95	117.00
33	BA	179	A	N9-C4-C5	5.90	108.16	105.80
1	AA	94	A	C8-N9-C4	5.90	108.16	105.80
1	AA	757	A	C4-C5-C6	5.90	119.95	117.00
1	AA	768	A	N3-C4-N9	5.90	132.12	127.40
1	AA	1333	A	N9-C4-C5	5.90	108.16	105.80
33	BA	882	A	C8-N9-C4	5.90	108.16	105.80
33	BA	1465	A	C4-C5-C6	5.90	119.95	117.00
33	BA	2141	A	C4-C5-C6	5.90	119.95	117.00
33	BA	2421	A	N3-C4-N9	5.90	132.12	127.40
1	AA	459	A	N3-C4-N9	5.90	132.12	127.40
1	AA	611	A	C4-C5-C6	5.90	119.95	117.00
1	AA	1456	A	C4-C5-C6	5.90	119.95	117.00
33	BA	477	A	N9-C4-C5	5.90	108.16	105.80
33	BA	1339	A	C8-N9-C4	5.90	108.16	105.80
33	BA	1784	A	C8-N9-C4	5.90	108.16	105.80
33	BA	2327	A	N3-C4-N9	5.90	132.12	127.40
33	BA	2338	A	N3-C4-N9	5.90	132.12	127.40
33	BA	2851	A	C4-C5-C6	5.90	119.95	117.00
1	AA	923	A	C8-N9-C4	5.90	108.16	105.80
33	BA	1375	A	C4-C5-C6	5.90	119.95	117.00
33	BA	1542	A	N3-C4-N9	5.90	132.12	127.40
33	BA	2810	A	C4-C5-C6	5.90	119.95	117.00
1	AA	518	A	N3-C4-N9	5.90	132.12	127.40
1	AA	823	A	C4-C5-C6	5.90	119.95	117.00
1	AA	828	A	N3-C4-N9	5.90	132.12	127.40
1	AA	1456	A	N3-C4-N9	5.90	132.12	127.40
33	BA	1029	A	N3-C4-N9	5.90	132.12	127.40
33	BA	1097	A	C4-C5-C6	5.90	119.95	117.00
33	BA	1243	A	C4-C5-C6	5.90	119.95	117.00
33	BA	1312	A	N3-C4-N9	5.90	132.12	127.40
33	BA	1723	A	N3-C4-N9	5.90	132.12	127.40
34	BB	76	A	N3-C4-N9	5.90	132.12	127.40
1	AA	254	A	C8-N9-C4	5.90	108.16	105.80
1	AA	1513	A	N3-C4-N9	5.90	132.12	127.40
33	BA	1202	A	C8-N9-C4	5.90	108.16	105.80
1	AA	485	A	C4-C5-C6	5.89	119.95	117.00
1	AA	500	A	N9-C4-C5	5.89	108.16	105.80
1	AA	919	A	N3-C4-N9	5.89	132.12	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1456	A	C8-N9-C4	5.89	108.16	105.80
33	BA	225	A	N3-C4-N9	5.89	132.12	127.40
33	BA	339	A	N3-C4-N9	5.89	132.12	127.40
33	BA	470	A	C4-C5-C6	5.89	119.95	117.00
33	BA	490	A	C8-N9-C4	5.89	108.16	105.80
33	BA	947	A	C4-C5-C6	5.89	119.95	117.00
33	BA	1141	A	C4-C5-C6	5.89	119.95	117.00
33	BA	2762	A	C4-C5-C6	5.89	119.95	117.00
1	AA	504	A	N3-C4-N9	5.89	132.11	127.40
1	AA	541	A	C4-C5-C6	5.89	119.95	117.00
1	AA	968	A	N3-C4-N9	5.89	132.11	127.40
1	AA	1197	A	N3-C4-N9	5.89	132.11	127.40
33	BA	278	A	N3-C4-N9	5.89	132.11	127.40
1	AA	225	A	N3-C4-N9	5.89	132.11	127.40
1	AA	532	A	N3-C4-N9	5.89	132.11	127.40
1	AA	762	A	N3-C4-N9	5.89	132.11	127.40
33	BA	2417	A	C8-N9-C4	5.89	108.16	105.80
34	BB	27	A	C4-C5-C6	5.89	119.95	117.00
1	AA	52	A	C4-C5-C6	5.89	119.94	117.00
1	AA	94	A	C4-C5-C6	5.89	119.94	117.00
1	AA	266	A	C4-C5-C6	5.89	119.94	117.00
1	AA	928	A	N3-C4-N9	5.89	132.11	127.40
1	AA	1298	A	N3-C4-N9	5.89	132.11	127.40
33	BA	71	A	C8-N9-C4	5.89	108.16	105.80
33	BA	236	A	N3-C4-N9	5.89	132.11	127.40
33	BA	646	A	C4-C5-C6	5.89	119.94	117.00
33	BA	653	A	C4-C5-C6	5.89	119.94	117.00
33	BA	746	A	C4-C5-C6	5.89	119.94	117.00
33	BA	782	A	C4-C5-C6	5.89	119.94	117.00
33	BA	1243	A	N3-C4-N9	5.89	132.11	127.40
33	BA	1745	A	N3-C4-N9	5.89	132.11	127.40
33	BA	1815	A	C4-C5-C6	5.89	119.94	117.00
33	BA	2330	A	N9-C4-C5	5.89	108.16	105.80
33	BA	2362	A	C8-N9-C4	5.89	108.16	105.80
33	BA	2661	A	N3-C4-N9	5.89	132.11	127.40
1	AA	664	A	N3-C4-N9	5.89	132.11	127.40
1	AA	975	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1056	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1225	A	C4-C5-C6	5.89	119.94	117.00
33	BA	2132	A	C4-C5-C6	5.89	119.94	117.00
33	BA	2845	A	N3-C4-N9	5.89	132.11	127.40
1	AA	290	A	C4-C5-C6	5.89	119.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	372	A	N3-C4-N9	5.89	132.11	127.40
1	AA	616	A	N3-C4-N9	5.89	132.11	127.40
1	AA	910	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1017	A	C4-C5-C6	5.89	119.94	117.00
1	AA	1210	A	C4-C5-C6	5.89	119.94	117.00
33	BA	139	A	C4-C5-C6	5.89	119.94	117.00
33	BA	553	A	C4-C5-C6	5.89	119.94	117.00
33	BA	1175	A	C4-C5-C6	5.89	119.94	117.00
33	BA	1224	A	C4-C5-C6	5.89	119.94	117.00
33	BA	1314	A	C4-C5-C6	5.89	119.94	117.00
33	BA	1580	A	N3-C4-N9	5.89	132.11	127.40
33	BA	1981	A	N3-C4-N9	5.89	132.11	127.40
33	BA	2087	A	N3-C4-N9	5.89	132.11	127.40
33	BA	2464	A	N3-C4-N9	5.89	132.11	127.40
33	BA	2834	A	N3-C4-N9	5.89	132.11	127.40
1	AA	361	A	C4-C5-C6	5.88	119.94	117.00
1	AA	371	A	N3-C4-N9	5.88	132.11	127.40
1	AA	674	A	C4-C5-N7	-5.88	107.76	110.70
1	AA	1128	A	N3-C4-N9	5.88	132.11	127.40
1	AA	1417	A	C4-C5-C6	5.88	119.94	117.00
33	BA	1654	A	C4-C5-C6	5.88	119.94	117.00
33	BA	1967	A	N3-C4-N9	5.88	132.11	127.40
33	BA	2643	A	N3-C4-N9	5.88	132.11	127.40
1	AA	1342	A	N3-C4-N9	5.88	132.11	127.40
33	BA	652	A	N3-C4-N9	5.88	132.11	127.40
33	BA	1179	A	N3-C4-N9	5.88	132.11	127.40
33	BA	1913	A	C4-C5-C6	5.88	119.94	117.00
33	BA	2902	A	N3-C4-N9	5.88	132.11	127.40
1	AA	120	A	C4-C5-C6	5.88	119.94	117.00
1	AA	828	A	C4-C5-C6	5.88	119.94	117.00
1	AA	959	A	N3-C4-N9	5.88	132.11	127.40
33	BA	144	A	N3-C4-N9	5.88	132.11	127.40
33	BA	229	A	C4-C5-C6	5.88	119.94	117.00
33	BA	421	A	N3-C4-N9	5.88	132.10	127.40
33	BA	876	A	N3-C4-N9	5.88	132.10	127.40
33	BA	1034	A	C4-C5-C6	5.88	119.94	117.00
33	BA	1989	A	N3-C4-N9	5.88	132.10	127.40
33	BA	2000	A	N3-C4-N9	5.88	132.10	127.40
33	BA	2907	A	N3-C4-N9	5.88	132.10	127.40
1	AA	786	A	N3-C4-N9	5.88	132.10	127.40
1	AA	1248	A	C8-N9-C4	5.88	108.15	105.80
1	AA	1451	A	N3-C4-N9	5.88	132.10	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	183	A	N9-C4-C5	5.88	108.15	105.80
33	BA	835	A	C8-N9-C4	5.88	108.15	105.80
33	BA	1995	A	N3-C4-N9	5.88	132.10	127.40
1	AA	886	A	N3-C4-N9	5.88	132.10	127.40
1	AA	1197	A	C4-C5-C6	5.88	119.94	117.00
33	BA	727	A	C4-C5-C6	5.88	119.94	117.00
33	BA	1254	A	N3-C4-N9	5.88	132.10	127.40
33	BA	1269	A	N3-C4-N9	5.88	132.10	127.40
33	BA	1323	A	N3-C4-N9	5.88	132.10	127.40
33	BA	1913	A	N3-C4-N9	5.88	132.10	127.40
33	BA	2170	A	N3-C4-N9	5.88	132.10	127.40
33	BA	2406	A	N3-C4-N9	5.88	132.10	127.40
33	BA	2860	A	N3-C4-N9	5.88	132.10	127.40
1	AA	372	A	C4-C5-C6	5.88	119.94	117.00
1	AA	544	A	C4-C5-C6	5.88	119.94	117.00
1	AA	1236	A	N3-C4-N9	5.88	132.10	127.40
1	AA	1523	A	N3-C4-N9	5.88	132.10	127.40
33	BA	1036	A	C4-C5-C6	5.88	119.94	117.00
33	BA	1126	A	C8-N9-C4	5.88	108.15	105.80
33	BA	2032	A	N3-C4-N9	5.88	132.10	127.40
33	BA	2034	A	N3-C4-N9	5.88	132.10	127.40
33	BA	2191	A	C4-C5-C6	5.88	119.94	117.00
34	BB	43	A	N3-C4-N9	5.88	132.10	127.40
1	AA	1271	A	N3-C4-N9	5.88	132.10	127.40
33	BA	231	A	N3-C4-N9	5.88	132.10	127.40
33	BA	1142	A	C4-C5-C6	5.88	119.94	117.00
33	BA	1679	A	C4-C5-C6	5.88	119.94	117.00
33	BA	2034	A	C4-C5-C6	5.88	119.94	117.00
33	BA	2767	A	C4-C5-C6	5.88	119.94	117.00
1	AA	12	A	N3-C4-N9	5.87	132.10	127.40
1	AA	389	A	N3-C4-N9	5.87	132.10	127.40
1	AA	1054	A	N3-C4-N9	5.87	132.10	127.40
1	AA	1120	A	C4-C5-C6	5.87	119.94	117.00
1	AA	1259	A	N3-C4-N9	5.87	132.10	127.40
33	BA	71	A	C4-C5-C6	5.87	119.94	117.00
33	BA	91	A	N3-C4-N9	5.87	132.10	127.40
33	BA	225	A	C4-C5-C6	5.87	119.94	117.00
33	BA	763	A	N3-C4-N9	5.87	132.10	127.40
33	BA	828	A	C4-C5-C6	5.87	119.94	117.00
33	BA	1014	A	C8-N9-C4	5.87	108.15	105.80
33	BA	1697	A	N3-C4-N9	5.87	132.10	127.40
33	BA	1967	A	C4-C5-C6	5.87	119.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	120	A	N3-C4-N9	5.87	132.10	127.40
1	AA	501	A	C4-C5-C6	5.87	119.94	117.00
1	AA	506	A	C4-C5-N7	-5.87	107.76	110.70
1	AA	677	A	C8-N9-C4	5.87	108.15	105.80
1	AA	870	A	C4-C5-N7	-5.87	107.76	110.70
1	AA	1111	A	C4-C5-C6	5.87	119.94	117.00
1	AA	1121	A	N3-C4-N9	5.87	132.10	127.40
1	AA	1180	A	N3-C4-N9	5.87	132.10	127.40
1	AA	1185	A	N3-C4-N9	5.87	132.10	127.40
1	AA	1386	A	C4-C5-C6	5.87	119.94	117.00
1	AA	1541	A	C4-C5-C6	5.87	119.94	117.00
33	BA	475	A	C4-C5-C6	5.87	119.94	117.00
33	BA	1210	A	N3-C4-N9	5.87	132.10	127.40
33	BA	1269	A	C4-C5-C6	5.87	119.94	117.00
33	BA	1291	A	C8-N9-C4	5.87	108.15	105.80
33	BA	1722	A	C4-C5-C6	5.87	119.94	117.00
33	BA	1802	A	N3-C4-N9	5.87	132.10	127.40
33	BA	1906	A	C4-C5-C6	5.87	119.94	117.00
33	BA	2155	A	C4-C5-C6	5.87	119.94	117.00
33	BA	548	A	N3-C4-N9	5.87	132.10	127.40
33	BA	1072	A	C4-C5-C6	5.87	119.94	117.00
33	BA	1221	A	N3-C4-N9	5.87	132.10	127.40
1	AA	423	A	C4-C5-C6	5.87	119.93	117.00
1	AA	556	A	C8-N9-C4	5.87	108.15	105.80
1	AA	685	A	N3-C4-N9	5.87	132.09	127.40
1	AA	724	A	N3-C4-N9	5.87	132.10	127.40
1	AA	776	A	C4-C5-C6	5.87	119.94	117.00
33	BA	161	A	N9-C4-C5	5.87	108.15	105.80
33	BA	659	A	N3-C4-N9	5.87	132.09	127.40
33	BA	851	A	N3-C4-N9	5.87	132.09	127.40
33	BA	922	A	N3-C4-N9	5.87	132.09	127.40
33	BA	1291	A	N3-C4-N9	5.87	132.09	127.40
33	BA	1302	A	N9-C4-C5	5.87	108.15	105.80
33	BA	1453	A	N3-C4-N9	5.87	132.09	127.40
33	BA	1631	A	N3-C4-N9	5.87	132.09	127.40
33	BA	1876	A	N3-C4-N9	5.87	132.09	127.40
33	BA	2152	A	C4-C5-C6	5.87	119.93	117.00
33	BA	2893	A	C4-C5-C6	5.87	119.93	117.00
1	AA	1403	A	N3-C4-N9	5.87	132.09	127.40
33	BA	281	A	C4-C5-N7	-5.87	107.77	110.70
33	BA	1113	A	N3-C4-N9	5.87	132.09	127.40
33	BA	1305	A	C8-N9-C4	5.87	108.15	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2007	A	C4-C5-C6	5.87	119.93	117.00
1	AA	491	A	N3-C4-N9	5.87	132.09	127.40
1	AA	1528	A	N3-C4-N9	5.87	132.09	127.40
33	BA	28	A	C8-N9-C4	5.87	108.15	105.80
33	BA	73	A	N3-C4-N9	5.87	132.09	127.40
33	BA	222	A	N3-C4-N9	5.87	132.09	127.40
33	BA	699	A	N3-C4-N9	5.87	132.09	127.40
33	BA	829	A	N3-C4-N9	5.87	132.09	127.40
33	BA	917	A	C4-C5-C6	5.87	119.93	117.00
33	BA	1347	A	N9-C4-C5	5.87	108.15	105.80
33	BA	1700	A	C4-C5-C6	5.87	119.93	117.00
33	BA	1838	A	N3-C4-N9	5.87	132.09	127.40
33	BA	1929	A	C4-C5-C6	5.87	119.93	117.00
33	BA	2007	A	N3-C4-N9	5.87	132.09	127.40
1	AA	423	A	N3-C4-N9	5.86	132.09	127.40
1	AA	799	A	N3-C4-N9	5.86	132.09	127.40
1	AA	925	A	C8-N9-C4	5.86	108.15	105.80
1	AA	1437	A	N3-C4-N9	5.86	132.09	127.40
1	AA	1466	A	C4-C5-C6	5.86	119.93	117.00
33	BA	65	A	N3-C4-N9	5.86	132.09	127.40
33	BA	110	A	N3-C4-N9	5.86	132.09	127.40
33	BA	519	A	N3-C4-N9	5.86	132.09	127.40
33	BA	553	A	N3-C4-N9	5.86	132.09	127.40
33	BA	600	A	N3-C4-N9	5.86	132.09	127.40
33	BA	1797	A	C4-C5-C6	5.86	119.93	117.00
33	BA	1965	A	N9-C4-C5	5.86	108.15	105.80
33	BA	2298	A	N3-C4-N9	5.86	132.09	127.40
33	BA	2708	A	N3-C4-N9	5.86	132.09	127.40
33	BA	2762	A	N3-C4-N9	5.86	132.09	127.40
1	AA	684	A	N3-C4-N9	5.86	132.09	127.40
1	AA	1048	A	C4-C5-C6	5.86	119.93	117.00
33	BA	867	A	N3-C4-N9	5.86	132.09	127.40
33	BA	2658	A	N3-C4-N9	5.86	132.09	127.40
1	AA	18	A	C8-N9-C4	5.86	108.14	105.80
1	AA	475	A	N3-C4-N9	5.86	132.09	127.40
1	AA	730	A	C4-C5-C6	5.86	119.93	117.00
1	AA	738	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1503	A	C4-C5-C6	5.86	119.93	117.00
33	BA	781	A	N3-C4-N9	5.86	132.09	127.40
33	BA	1464	A	N3-C4-N9	5.86	132.09	127.40
33	BA	1918	A	N3-C4-N9	5.86	132.09	127.40
33	BA	1930	A	N3-C4-N9	5.86	132.09	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1942	A	N3-C4-N9	5.86	132.09	127.40
33	BA	2777	A	C8-N9-C4	5.86	108.14	105.80
34	BB	25	A	C8-N9-C4	5.86	108.14	105.80
1	AA	669	A	N3-C4-N9	5.86	132.09	127.40
1	AA	690	A	C4-C5-C6	5.86	119.93	117.00
1	AA	522	A	N3-C4-N9	5.86	132.09	127.40
1	AA	777	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1102	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1176	A	N3-C4-N9	5.86	132.09	127.40
1	AA	1510	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1529	A	N3-C4-N9	5.86	132.09	127.40
33	BA	281	A	N9-C4-C5	5.86	108.14	105.80
33	BA	421	A	C8-N9-C4	5.86	108.14	105.80
33	BA	477	A	C4-C5-C6	5.86	119.93	117.00
33	BA	525	A	C4-C5-C6	5.86	119.93	117.00
33	BA	1072	A	N3-C4-N9	5.86	132.09	127.40
33	BA	1982	A	C8-N9-C4	5.86	108.14	105.80
33	BA	2155	A	C8-N9-C4	5.86	108.14	105.80
33	BA	2317	A	N3-C4-N9	5.86	132.09	127.40
33	BA	2770	A	N3-C4-N9	5.86	132.09	127.40
34	BB	105	A	N3-C4-N9	5.86	132.09	127.40
34	BB	114	A	N3-C4-N9	5.86	132.09	127.40
1	AA	389	A	C4-C5-C6	5.86	119.93	117.00
1	AA	1200	A	N3-C4-N9	5.86	132.08	127.40
33	BA	150	A	C8-N9-C4	5.86	108.14	105.80
33	BA	220	A	N3-C4-N9	5.86	132.08	127.40
33	BA	302	A	C4-C5-C6	5.86	119.93	117.00
33	BA	436	A	N3-C4-N9	5.86	132.08	127.40
33	BA	1308	A	N3-C4-N9	5.86	132.08	127.40
33	BA	1313	A	N3-C4-N9	5.86	132.09	127.40
33	BA	1347	A	C4-C5-N7	-5.86	107.77	110.70
33	BA	2387	A	N3-C4-N9	5.86	132.08	127.40
33	BA	2740	A	N3-C4-N9	5.86	132.08	127.40
1	AA	457	A	N9-C4-C5	5.85	108.14	105.80
1	AA	1434	A	C8-N9-C4	5.85	108.14	105.80
33	BA	247	A	C4-C5-C6	5.85	119.93	117.00
33	BA	547	A	N3-C4-N9	5.85	132.08	127.40
33	BA	835	A	C4-C5-C6	5.85	119.93	117.00
33	BA	1116	A	N3-C4-N9	5.85	132.08	127.40
33	BA	1405	A	N3-C4-N9	5.85	132.08	127.40
33	BA	2083	A	N3-C4-N9	5.85	132.08	127.40
1	AA	555	A	N3-C4-N9	5.85	132.08	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1031	A	N3-C4-N9	5.85	132.08	127.40
1	AA	1225	A	C8-N9-C4	5.85	108.14	105.80
33	BA	199	A	C4-C5-C6	5.85	119.93	117.00
33	BA	333	A	N3-C4-N9	5.85	132.08	127.40
33	BA	561	A	N3-C4-N9	5.85	132.08	127.40
33	BA	677	A	C4-C5-C6	5.85	119.93	117.00
33	BA	770	A	N3-C4-N9	5.85	132.08	127.40
33	BA	1406	A	N3-C4-N9	5.85	132.08	127.40
33	BA	1540	A	C4-C5-C6	5.85	119.93	117.00
33	BA	1553	A	C4-C5-C6	5.85	119.93	117.00
33	BA	1809	A	C4-C5-C6	5.85	119.93	117.00
33	BA	2030	A	C4-C5-C6	5.85	119.93	117.00
33	BA	2769	A	N3-C4-N9	5.85	132.08	127.40
33	BA	2835	A	C4-C5-C6	5.85	119.93	117.00
1	AA	206	A	C8-N9-C4	5.85	108.14	105.80
1	AA	258	A	N3-C4-N9	5.85	132.08	127.40
1	AA	979	A	N3-C4-N9	5.85	132.08	127.40
33	BA	53	A	C4-C5-C6	5.85	119.93	117.00
33	BA	322	A	C4-C5-C6	5.85	119.92	117.00
33	BA	1677	A	C4-C5-C6	5.85	119.93	117.00
1	AA	507	A	C8-N9-C4	5.85	108.14	105.80
33	BA	10	A	N3-C4-N9	5.85	132.08	127.40
33	BA	150	A	N3-C4-N9	5.85	132.08	127.40
33	BA	1055	A	N3-C4-N9	5.85	132.08	127.40
34	BB	56	A	N3-C4-N9	5.85	132.08	127.40
1	AA	422	A	C4-C5-C6	5.85	119.92	117.00
1	AA	581	A	C4-C5-C6	5.85	119.92	117.00
1	AA	672	A	C8-N9-C4	5.85	108.14	105.80
1	AA	823	A	N3-C4-N9	5.85	132.08	127.40
1	AA	1056	A	N3-C4-N9	5.85	132.08	127.40
1	AA	1479	A	N3-C4-N9	5.85	132.08	127.40
21	AX	14	A	C4-C5-C6	5.85	119.92	117.00
33	BA	53	A	N3-C4-N9	5.85	132.08	127.40
33	BA	325	A	C4-C5-C6	5.85	119.92	117.00
33	BA	428	A	N3-C4-N9	5.85	132.08	127.40
33	BA	1305	A	N9-C4-C5	5.85	108.14	105.80
33	BA	2860	A	C4-C5-C6	5.85	119.92	117.00
1	AA	1147	A	N3-C4-N9	5.85	132.08	127.40
33	BA	325	A	N3-C4-N9	5.85	132.08	127.40
33	BA	1533	A	C4-C5-C6	5.85	119.92	117.00
33	BA	1593	A	N3-C4-N9	5.85	132.08	127.40
1	AA	67	A	N3-C4-N9	5.84	132.07	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	94	A	N3-C4-N9	5.84	132.08	127.40
33	BA	637	A	N3-C4-N9	5.84	132.07	127.40
33	BA	786	A	N3-C4-N9	5.84	132.08	127.40
33	BA	811	A	N9-C4-C5	5.84	108.14	105.80
33	BA	958	A	N3-C4-N9	5.84	132.08	127.40
33	BA	1346	A	N3-C4-N9	5.84	132.08	127.40
33	BA	1540	A	N3-C4-N9	5.84	132.07	127.40
33	BA	1713	A	C8-N9-C4	5.84	108.14	105.80
33	BA	2898	A	N9-C4-C5	5.84	108.14	105.80
34	BB	113	A	C4-C5-C6	5.84	119.92	117.00
1	AA	139	A	N3-C4-N9	5.84	132.07	127.40
1	AA	477	A	N3-C4-N9	5.84	132.07	127.40
1	AA	910	A	N3-C4-N9	5.84	132.07	127.40
33	BA	2912	A	C4-C5-C6	5.84	119.92	117.00
34	BB	17	A	C4-C5-C6	5.84	119.92	117.00
1	AA	178	A	C4-C5-C6	5.84	119.92	117.00
1	AA	333	A	C4-C5-C6	5.84	119.92	117.00
1	AA	704	A	C4-C5-C6	5.84	119.92	117.00
1	AA	1028	A	N3-C4-N9	5.84	132.07	127.40
1	AA	1120	A	N3-C4-N9	5.84	132.07	127.40
33	BA	578	A	C8-N9-C4	5.84	108.14	105.80
33	BA	935	A	C4-C5-N7	-5.84	107.78	110.70
33	BA	1026	A	N3-C4-N9	5.84	132.07	127.40
33	BA	1078	A	C4-C5-N7	-5.84	107.78	110.70
33	BA	1115	A	C4-C5-C6	5.84	119.92	117.00
33	BA	1335	A	C4-C5-C6	5.84	119.92	117.00
33	BA	1339	A	C4-C5-C6	5.84	119.92	117.00
33	BA	1648	A	C8-N9-C4	5.84	108.14	105.80
33	BA	1686	A	N3-C4-N9	5.84	132.07	127.40
33	BA	1699	A	C4-C5-C6	5.84	119.92	117.00
33	BA	2146	A	N3-C4-N9	5.84	132.07	127.40
33	BA	2296	A	C4-C5-C6	5.84	119.92	117.00
1	AA	1185	A	C8-N9-C4	5.84	108.14	105.80
1	AA	1188	A	C4-C5-C6	5.84	119.92	117.00
33	BA	5	A	N3-C4-N9	5.84	132.07	127.40
33	BA	124	A	N3-C4-N9	5.84	132.07	127.40
33	BA	125	A	N9-C4-C5	5.84	108.14	105.80
33	BA	1046	A	N3-C4-N9	5.84	132.07	127.40
33	BA	1202	A	C4-C5-C6	5.84	119.92	117.00
33	BA	1381	A	N3-C4-N9	5.84	132.07	127.40
33	BA	1961	A	C4-C5-C6	5.84	119.92	117.00
33	BA	2059	A	C4-C5-C6	5.84	119.92	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2390	A	C4-C5-C6	5.84	119.92	117.00
33	BA	2440	A	N3-C4-N9	5.84	132.07	127.40
33	BA	2686	A	C4-C5-C6	5.84	119.92	117.00
1	AA	1320	A	N3-C4-N9	5.84	132.07	127.40
33	BA	1131	A	C8-N9-C4	5.84	108.14	105.80
33	BA	1314	A	C8-N9-C4	5.84	108.14	105.80
33	BA	1520	A	C8-N9-C4	5.84	108.14	105.80
33	BA	2256	A	N3-C4-N9	5.84	132.07	127.40
33	BA	2356	A	N3-C4-N9	5.84	132.07	127.40
1	AA	333	A	N3-C4-N9	5.84	132.07	127.40
33	BA	2455	A	C8-N9-C4	5.84	108.14	105.80
1	AA	485	A	N3-C4-N9	5.83	132.07	127.40
33	BA	139	A	N3-C4-N9	5.83	132.07	127.40
33	BA	1381	A	C4-C5-C6	5.83	119.92	117.00
33	BA	1832	A	N3-C4-N9	5.83	132.07	127.40
33	BA	1901	A	C8-N9-C4	5.83	108.13	105.80
33	BA	1967	A	C8-N9-C4	5.83	108.13	105.80
33	BA	2088	A	C4-C5-C6	5.83	119.92	117.00
33	BA	2088	A	C8-N9-C4	5.83	108.13	105.80
33	BA	2297	A	N3-C4-N9	5.83	132.07	127.40
1	AA	142	A	C4-C5-C6	5.83	119.92	117.00
1	AA	870	A	N9-C4-C5	5.83	108.13	105.80
1	AA	1090	A	C4-C5-C6	5.83	119.92	117.00
1	AA	1419	A	C4-C5-C6	5.83	119.92	117.00
33	BA	216	A	C8-N9-C4	5.83	108.13	105.80
33	BA	894	A	N3-C4-N9	5.83	132.07	127.40
33	BA	2134	A	C4-C5-N7	-5.83	107.78	110.70
33	BA	2315	A	C8-N9-C4	5.83	108.13	105.80
33	BA	2860	A	C8-N9-C4	5.83	108.13	105.80
33	BA	2923	A	N3-C4-N9	5.83	132.07	127.40
1	AA	118	A	C8-N9-C4	5.83	108.13	105.80
1	AA	211	A	N3-C4-N9	5.83	132.07	127.40
1	AA	532	A	C8-N9-C4	5.83	108.13	105.80
1	AA	801	A	N3-C4-N9	5.83	132.06	127.40
1	AA	975	A	C8-N9-C4	5.83	108.13	105.80
1	AA	1056	A	C8-N9-C4	5.83	108.13	105.80
1	AA	1103	A	N3-C4-N9	5.83	132.06	127.40
1	AA	1115	A	N3-C4-N9	5.83	132.07	127.40
1	AA	1185	A	C4-C5-C6	5.83	119.92	117.00
33	BA	1335	A	N3-C4-N9	5.83	132.07	127.40
33	BA	1734	A	N3-C4-N9	5.83	132.07	127.40
33	BA	1788	A	N3-C4-N9	5.83	132.07	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1925	A	C8-N9-C4	5.83	108.13	105.80
1	AA	107	A	N3-C4-N9	5.83	132.06	127.40
1	AA	206	A	C4-C5-C6	5.83	119.91	117.00
1	AA	306	A	C4-C5-C6	5.83	119.91	117.00
1	AA	321	A	C4-C5-C6	5.83	119.91	117.00
1	AA	456	A	C4-C5-C6	5.83	119.91	117.00
33	BA	653	A	N3-C4-N9	5.83	132.06	127.40
33	BA	987	A	N3-C4-N9	5.83	132.06	127.40
33	BA	1722	A	N3-C4-N9	5.83	132.06	127.40
33	BA	2060	A	N3-C4-N9	5.83	132.06	127.40
33	BA	2673	A	C4-C5-C6	5.83	119.92	117.00
33	BA	2683	A	C8-N9-C4	5.83	108.13	105.80
1	AA	287	A	N3-C4-N9	5.83	132.06	127.40
1	AA	419	A	C8-N9-C4	5.83	108.13	105.80
1	AA	803	A	N3-C4-N9	5.83	132.06	127.40
1	AA	1200	A	C4-C5-C6	5.83	119.91	117.00
33	BA	619	A	N3-C4-N9	5.83	132.06	127.40
33	BA	1654	A	C8-N9-C4	5.83	108.13	105.80
33	BA	2006	A	N3-C4-N9	5.83	132.06	127.40
33	BA	2447	A	C4-C5-C6	5.83	119.91	117.00
1	AA	142	A	N3-C4-N9	5.83	132.06	127.40
1	AA	386	A	C8-N9-C4	5.83	108.13	105.80
1	AA	978	A	N3-C4-N9	5.83	132.06	127.40
1	AA	1466	A	N3-C4-N9	5.83	132.06	127.40
33	BA	364	A	N3-C4-N9	5.83	132.06	127.40
33	BA	1149	A	C4-C5-C6	5.83	119.91	117.00
33	BA	1277	A	N3-C4-N9	5.83	132.06	127.40
33	BA	1724	A	N3-C4-N9	5.83	132.06	127.40
33	BA	1735	A	N3-C4-N9	5.83	132.06	127.40
33	BA	1895	A	C8-N9-C4	5.83	108.13	105.80
33	BA	2091	A	N3-C4-N9	5.83	132.06	127.40
33	BA	2606	A	C4-C5-N7	-5.83	107.79	110.70
33	BA	2670	A	C4-C5-N7	-5.83	107.79	110.70
1	AA	228	A	C4-C5-C6	5.82	119.91	117.00
1	AA	899	A	N9-C4-C5	5.82	108.13	105.80
1	AA	1355	A	N9-C4-C5	5.82	108.13	105.80
33	BA	219	A	C4-C5-C6	5.82	119.91	117.00
33	BA	1746	A	C4-C5-C6	5.82	119.91	117.00
33	BA	2869	A	N3-C4-N9	5.82	132.06	127.40
1	AA	974	A	C4-C5-C6	5.82	119.91	117.00
33	BA	1084	A	C4-C5-C6	5.82	119.91	117.00
33	BA	2719	A	C8-N9-C4	5.82	108.13	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	352	A	N3-C4-N9	5.82	132.06	127.40
1	AA	618	A	N3-C4-N9	5.82	132.06	127.40
1	AA	824	A	C8-N9-C4	5.82	108.13	105.80
1	AA	1333	A	C4-C5-N7	-5.82	107.79	110.70
33	BA	28	A	N3-C4-N9	5.82	132.06	127.40
33	BA	274	A	C4-C5-C6	5.82	119.91	117.00
33	BA	373	A	N3-C4-N9	5.82	132.06	127.40
33	BA	1097	A	N3-C4-N9	5.82	132.06	127.40
33	BA	1677	A	N3-C4-N9	5.82	132.06	127.40
33	BA	2837	A	N3-C4-N9	5.82	132.06	127.40
1	AA	189	A	C4-C5-C6	5.82	119.91	117.00
1	AA	638	A	N3-C4-N9	5.82	132.06	127.40
1	AA	1225	A	N3-C4-N9	5.82	132.06	127.40
33	BA	479	A	N3-C4-N9	5.82	132.06	127.40
33	BA	1230	A	N3-C4-N9	5.82	132.06	127.40
33	BA	2083	A	C8-N9-C4	5.82	108.13	105.80
1	AA	142	A	C8-N9-C4	5.82	108.13	105.80
1	AA	542	A	C4-C5-C6	5.82	119.91	117.00
1	AA	1451	A	C4-C5-C6	5.82	119.91	117.00
33	BA	618	A	N9-C4-C5	5.82	108.13	105.80
33	BA	619	A	C8-N9-C4	5.82	108.13	105.80
33	BA	1014	A	N3-C4-N9	5.82	132.05	127.40
33	BA	1144	A	N3-C4-N9	5.82	132.05	127.40
33	BA	1789	A	N3-C4-N9	5.82	132.05	127.40
33	BA	2594	A	N3-C4-N9	5.82	132.05	127.40
33	BA	2810	A	N3-C4-N9	5.82	132.05	127.40
33	BA	2876	A	N3-C4-N9	5.82	132.05	127.40
34	BB	25	A	C4-C5-C6	5.82	119.91	117.00
1	AA	62	A	N3-C4-N9	5.82	132.05	127.40
1	AA	204	A	N3-C4-N9	5.82	132.05	127.40
1	AA	281	A	N3-C4-N9	5.82	132.05	127.40
33	BA	543	A	N3-C4-N9	5.82	132.05	127.40
33	BA	1504	A	C4-C5-C6	5.82	119.91	117.00
33	BA	1533	A	N3-C4-N9	5.82	132.05	127.40
33	BA	1553	A	N3-C4-N9	5.82	132.05	127.40
33	BA	2042	A	C4-C5-C6	5.82	119.91	117.00
33	BA	2571	A	N3-C4-N9	5.82	132.05	127.40
33	BA	2875	A	N3-C4-N9	5.82	132.05	127.40
33	BA	2904	A	N3-C4-N9	5.82	132.05	127.40
1	AA	236	A	C4-C5-C6	5.81	119.91	117.00
1	AA	271	A	N3-C4-N9	5.81	132.05	127.40
1	AA	460	A	N3-C4-N9	5.81	132.05	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1298	A	C4-C5-C6	5.81	119.91	117.00
33	BA	1743	A	N3-C4-N9	5.81	132.05	127.40
33	BA	1746	A	N3-C4-N9	5.81	132.05	127.40
33	BA	1966	A	C4-C5-C6	5.81	119.91	117.00
33	BA	1998	A	C8-N9-C4	5.81	108.13	105.80
33	BA	2216	A	N3-C4-N9	5.81	132.05	127.40
1	AA	947	A	N3-C4-N9	5.81	132.05	127.40
1	AA	1342	A	C4-C5-C6	5.81	119.91	117.00
33	BA	84	A	N3-C4-N9	5.81	132.05	127.40
33	BA	178	A	N9-C4-C5	5.81	108.12	105.80
33	BA	782	A	N3-C4-N9	5.81	132.05	127.40
33	BA	1078	A	C4-C5-C6	5.81	119.91	117.00
33	BA	1308	A	C4-C5-C6	5.81	119.91	117.00
33	BA	1504	A	N3-C4-N9	5.81	132.05	127.40
33	BA	1592	A	N3-C4-N9	5.81	132.05	127.40
33	BA	2606	A	N9-C4-C5	5.81	108.12	105.80
34	BB	55	A	N3-C4-N9	5.81	132.05	127.40
1	AA	251	A	N3-C4-N9	5.81	132.05	127.40
1	AA	1488	A	C4-C5-C6	5.81	119.91	117.00
1	AA	361	A	C8-N9-C4	5.81	108.12	105.80
1	AA	440	A	N3-C4-N9	5.81	132.05	127.40
1	AA	500	A	C4-C5-C6	5.81	119.91	117.00
33	BA	56	A	C8-N9-C4	5.81	108.12	105.80
33	BA	324	A	C4-C5-C6	5.81	119.90	117.00
33	BA	828	A	N3-C4-N9	5.81	132.05	127.40
33	BA	1189	A	C8-N9-C4	5.81	108.12	105.80
1	AA	190	A	N3-C4-N9	5.81	132.05	127.40
1	AA	1248	A	N3-C4-N9	5.81	132.05	127.40
33	BA	166	A	C4-C5-C6	5.81	119.90	117.00
33	BA	727	A	N3-C4-N9	5.81	132.05	127.40
33	BA	978	A	N3-C4-N9	5.81	132.05	127.40
33	BA	1224	A	N3-C4-N9	5.81	132.05	127.40
33	BA	2526	A	N3-C4-N9	5.81	132.05	127.40
33	BA	2686	A	N3-C4-N9	5.81	132.05	127.40
1	AA	583	A	N9-C4-C5	5.81	108.12	105.80
33	BA	575	A	C8-N9-C4	5.81	108.12	105.80
33	BA	1417	A	C8-N9-C4	5.81	108.12	105.80
33	BA	2071	A	C4-C5-C6	5.81	119.90	117.00
33	BA	2447	A	C8-N9-C4	5.81	108.12	105.80
34	BB	51	A	C8-N9-C4	5.81	108.12	105.80
1	AA	160	A	N3-C4-N9	5.80	132.04	127.40
1	AA	367	A	C4-C5-C6	5.80	119.90	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	651	A	C4-C5-C6	5.80	119.90	117.00
1	AA	786	A	C8-N9-C4	5.80	108.12	105.80
1	AA	1210	A	N3-C4-N9	5.80	132.04	127.40
1	AA	1372	A	C4-C5-N7	-5.80	107.80	110.70
33	BA	677	A	N3-C4-N9	5.80	132.04	127.40
33	BA	2390	A	N3-C4-N9	5.80	132.04	127.40
1	AA	440	A	C4-C5-C6	5.80	119.90	117.00
1	AA	1188	A	C8-N9-C4	5.80	108.12	105.80
33	BA	1036	A	N3-C4-N9	5.80	132.04	127.40
33	BA	1464	A	C8-N9-C4	5.80	108.12	105.80
33	BA	1534	A	N3-C4-N9	5.80	132.04	127.40
1	AA	439	A	N9-C4-C5	5.80	108.12	105.80
1	AA	544	A	N3-C4-N9	5.80	132.04	127.40
1	AA	1140	A	N3-C4-N9	5.80	132.04	127.40
1	AA	1261	A	N3-C4-N9	5.80	132.04	127.40
1	AA	1266	A	N3-C4-N9	5.80	132.04	127.40
33	BA	176	A	C4-C5-C6	5.80	119.90	117.00
33	BA	374	A	C8-N9-C4	5.80	108.12	105.80
33	BA	389	A	C4-C5-C6	5.80	119.90	117.00
33	BA	618	A	C4-C5-N7	-5.80	107.80	110.70
33	BA	2447	A	N3-C4-N9	5.80	132.04	127.40
33	BA	2779	A	N3-C4-N9	5.80	132.04	127.40
33	BA	2923	A	C8-N9-C4	5.80	108.12	105.80
34	BB	113	A	N3-C4-N9	5.80	132.04	127.40
1	AA	460	A	C8-N9-C4	5.80	108.12	105.80
1	AA	474	A	N3-C4-N9	5.80	132.04	127.40
1	AA	1213	A	C4-C5-C6	5.80	119.90	117.00
1	AA	1443	A	C4-C5-C6	5.80	119.90	117.00
1	AA	1466	A	C8-N9-C4	5.80	108.12	105.80
33	BA	281	A	N3-C4-N9	5.80	132.04	127.40
33	BA	1092	A	C4-C5-C6	5.80	119.90	117.00
33	BA	2018	A	N3-C4-N9	5.80	132.04	127.40
33	BA	2132	A	N3-C4-N9	5.80	132.04	127.40
33	BA	2340	A	N3-C4-N9	5.80	132.04	127.40
33	BA	2390	A	C8-N9-C4	5.80	108.12	105.80
33	BA	273	A	N9-C4-C5	5.80	108.12	105.80
33	BA	504	A	N9-C4-C5	5.80	108.12	105.80
33	BA	965	A	N3-C4-N9	5.80	132.04	127.40
1	AA	757	A	N3-C4-N9	5.80	132.04	127.40
1	AA	1197	A	C8-N9-C4	5.80	108.12	105.80
33	BA	418	A	N3-C4-N9	5.80	132.04	127.40
33	BA	736	A	C5-C6-N1	5.80	120.60	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	893	A	N3-C4-N9	5.80	132.04	127.40
33	BA	2254	A	N9-C4-C5	5.80	108.12	105.80
33	BA	2417	A	N3-C4-N9	5.80	132.04	127.40
1	AA	988	A	C4-C5-N7	-5.79	107.80	110.70
33	BA	476	A	C4-C5-C6	5.79	119.90	117.00
33	BA	1314	A	N3-C4-N9	5.79	132.04	127.40
33	BA	1699	A	N3-C4-N9	5.79	132.04	127.40
1	AA	258	A	C4-C5-C6	5.79	119.90	117.00
1	AA	463	A	N3-C4-N9	5.79	132.03	127.40
1	AA	592	A	N3-C4-N9	5.79	132.03	127.40
1	AA	704	A	N3-C4-N9	5.79	132.03	127.40
1	AA	1111	A	N3-C4-N9	5.79	132.03	127.40
1	AA	1207	A	C4-C5-C6	5.79	119.90	117.00
1	AA	1355	A	C8-N9-C4	5.79	108.12	105.80
1	AA	1386	A	C8-N9-C4	5.79	108.12	105.80
33	BA	1189	A	C4-C5-C6	5.79	119.90	117.00
33	BA	1326	A	N3-C4-N9	5.79	132.04	127.40
33	BA	1850	A	N3-C4-N9	5.79	132.03	127.40
33	BA	2876	A	C8-N9-C4	5.79	108.12	105.80
1	AA	53	A	N3-C4-N9	5.79	132.03	127.40
1	AA	768	A	C8-N9-C4	5.79	108.12	105.80
1	AA	1205	A	N3-C4-N9	5.79	132.03	127.40
33	BA	176	A	N3-C4-N9	5.79	132.03	127.40
33	BA	667	A	N9-C4-C5	5.79	108.12	105.80
33	BA	876	A	C8-N9-C4	5.79	108.12	105.80
33	BA	1020	A	C4-C5-C6	5.79	119.90	117.00
33	BA	1302	A	C4-C5-N7	-5.79	107.81	110.70
33	BA	2059	A	N3-C4-N9	5.79	132.03	127.40
33	BA	2923	A	C4-C5-C6	5.79	119.89	117.00
34	BB	39	A	N3-C4-N9	5.79	132.03	127.40
1	AA	107	A	C8-N9-C4	5.79	108.12	105.80
1	AA	386	A	C4-C5-C6	5.79	119.89	117.00
1	AA	569	A	C4-C5-C6	5.79	119.89	117.00
1	AA	696	A	C8-N9-C4	5.79	108.12	105.80
33	BA	1034	A	N3-C4-N9	5.79	132.03	127.40
33	BA	2807	A	C4-C5-N7	-5.79	107.81	110.70
1	AA	568	A	C8-N9-C4	5.79	108.12	105.80
1	AA	776	A	N3-C4-N9	5.79	132.03	127.40
1	AA	811	A	C8-N9-C4	5.79	108.11	105.80
1	AA	1503	A	C8-N9-C4	5.79	108.12	105.80
33	BA	198	A	N3-C4-N9	5.79	132.03	127.40
33	BA	314	A	C8-N9-C4	5.79	108.12	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1142	A	N3-C4-N9	5.79	132.03	127.40
33	BA	1325	A	C8-N9-C4	5.79	108.11	105.80
33	BA	1516	A	N3-C4-N9	5.79	132.03	127.40
34	BB	27	A	N3-C4-N9	5.79	132.03	127.40
1	AA	290	A	N3-C4-N9	5.79	132.03	127.40
1	AA	1050	A	C4-C5-C6	5.79	119.89	117.00
1	AA	1257	A	N3-C4-N9	5.79	132.03	127.40
33	BA	1423	A	N3-C4-N9	5.79	132.03	127.40
33	BA	1465	A	N3-C4-N9	5.79	132.03	127.40
33	BA	2851	A	C8-N9-C4	5.79	108.11	105.80
1	AA	159	A	C8-N9-C4	5.79	108.11	105.80
1	AA	862	A	C8-N9-C4	5.79	108.11	105.80
1	AA	899	A	C8-N9-C4	5.79	108.11	105.80
1	AA	1176	A	C8-N9-C4	5.79	108.11	105.80
1	AA	1320	A	C4-C5-N7	-5.79	107.81	110.70
33	BA	14	A	N3-C4-N9	5.79	132.03	127.40
33	BA	219	A	N3-C4-N9	5.79	132.03	127.40
33	BA	717	A	C4-C5-C6	5.79	119.89	117.00
33	BA	1149	A	N3-C4-N9	5.79	132.03	127.40
33	BA	1173	A	N9-C1'-C2'	5.79	121.52	114.00
33	BA	1244	A	N3-C4-N9	5.79	132.03	127.40
33	BA	2507	A	C4-C5-C6	5.79	119.89	117.00
33	BA	2810	A	C8-N9-C4	5.79	108.11	105.80
33	BA	2912	A	N3-C4-N9	5.79	132.03	127.40
1	AA	120	A	C8-N9-C4	5.78	108.11	105.80
1	AA	202	A	C4-C5-C6	5.78	119.89	117.00
1	AA	923	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1210	A	C8-N9-C4	5.78	108.11	105.80
1	AA	1502	A	N3-C4-N9	5.78	132.03	127.40
33	BA	345	A	C4-C5-C6	5.78	119.89	117.00
33	BA	1066	A	N3-C4-N9	5.78	132.03	127.40
33	BA	1906	A	N3-C4-N9	5.78	132.03	127.40
33	BA	2807	A	N9-C4-C5	5.78	108.11	105.80
1	AA	568	A	N3-C4-N9	5.78	132.03	127.40
33	BA	2152	A	N3-C4-N9	5.78	132.03	127.40
34	BB	44	A	N3-C4-N9	5.78	132.03	127.40
1	AA	240	A	N3-C4-N9	5.78	132.03	127.40
1	AA	988	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1090	A	C8-N9-C4	5.78	108.11	105.80
33	BA	216	A	C4-C5-C6	5.78	119.89	117.00
33	BA	448	A	N3-C4-N9	5.78	132.02	127.40
33	BA	683	A	C4-C5-C6	5.78	119.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	947	A	C8-N9-C4	5.78	108.11	105.80
33	BA	1020	A	N3-C4-N9	5.78	132.03	127.40
33	BA	2134	A	N9-C4-C5	5.78	108.11	105.80
33	BA	2670	A	C8-N9-C4	5.78	108.11	105.80
34	BB	39	A	C4-C5-C6	5.78	119.89	117.00
1	AA	236	A	N3-C4-N9	5.78	132.02	127.40
1	AA	357	A	N3-C4-N9	5.78	132.02	127.40
33	BA	126	A	C8-N9-C4	5.78	108.11	105.80
33	BA	210	A	C4-C5-C6	5.78	119.89	117.00
33	BA	470	A	N3-C4-N9	5.78	132.02	127.40
33	BA	908	A	N3-C4-N9	5.78	132.02	127.40
34	BB	18	A	N3-C4-N9	5.78	132.02	127.40
1	AA	335	A	C8-N9-C4	5.78	108.11	105.80
1	AA	605	A	C8-N9-C4	5.78	108.11	105.80
1	AA	1328	A	N3-C4-N9	5.78	132.02	127.40
1	AA	1510	A	N3-C4-N9	5.78	132.02	127.40
33	BA	343	A	N3-C4-N9	5.78	132.02	127.40
33	BA	736	A	C8-N9-C4	5.78	108.11	105.80
33	BA	1056	A	N9-C4-C5	5.78	108.11	105.80
33	BA	1813	A	C8-N9-C4	5.78	108.11	105.80
33	BA	1844	A	N9-C4-C5	5.78	108.11	105.80
33	BA	2303	A	N3-C4-N9	5.78	132.02	127.40
1	AA	730	A	C8-N9-C4	5.78	108.11	105.80
1	AA	1256	A	C8-N9-C4	5.78	108.11	105.80
33	BA	229	A	N3-C4-N9	5.78	132.02	127.40
33	BA	572	A	C4-C5-C6	5.78	119.89	117.00
33	BA	765	A	N9-C4-C5	5.78	108.11	105.80
33	BA	835	A	N3-C4-N9	5.78	132.02	127.40
33	BA	1287	A	C4-C5-C6	5.78	119.89	117.00
33	BA	2262	A	C4-C5-N7	-5.78	107.81	110.70
33	BA	2542	A	N3-C4-N9	5.78	132.02	127.40
34	BB	99	A	C5-C6-N1	5.78	120.59	117.70
1	AA	1006	A	C4-C5-C6	5.77	119.89	117.00
33	BA	117	A	N3-C4-N9	5.77	132.02	127.40
33	BA	475	A	N3-C4-N9	5.77	132.02	127.40
33	BA	646	A	N3-C4-N9	5.77	132.02	127.40
33	BA	2673	A	N3-C4-N9	5.77	132.02	127.40
1	AA	401	A	C4-C5-C6	5.77	119.89	117.00
1	AA	617	A	C8-N9-C4	5.77	108.11	105.80
1	AA	725	A	N9-C4-C5	5.77	108.11	105.80
33	BA	526	A	C8-N9-C4	5.77	108.11	105.80
33	BA	582	A	C8-N9-C4	5.77	108.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	746	A	N3-C4-N9	5.77	132.02	127.40
33	BA	1473	A	N9-C4-C5	5.77	108.11	105.80
33	BA	2049	A	C4-C5-N7	-5.77	107.81	110.70
33	BA	2062	A	C4-C5-N7	-5.77	107.81	110.70
33	BA	2455	A	C4-C5-C6	5.77	119.89	117.00
33	BA	2606	A	C4-C5-C6	5.77	119.89	117.00
1	AA	266	A	N9-C4-C5	5.77	108.11	105.80
1	AA	296	A	N3-C4-N9	5.77	132.02	127.40
1	AA	730	A	N3-C4-N9	5.77	132.02	127.40
1	AA	975	A	N3-C4-N9	5.77	132.02	127.40
33	BA	808	A	C8-N9-C4	5.77	108.11	105.80
33	BA	1553	A	C8-N9-C4	5.77	108.11	105.80
1	AA	170	A	N9-C4-C5	5.77	108.11	105.80
1	AA	346	A	C8-N9-C4	5.77	108.11	105.80
33	BA	84	A	C4-C5-C6	5.77	119.88	117.00
33	BA	412	A	C8-N9-C4	5.77	108.11	105.80
33	BA	724	A	C8-N9-C4	5.77	108.11	105.80
33	BA	1161	A	C4-C5-C6	5.77	119.89	117.00
33	BA	2141	A	N9-C4-C5	5.77	108.11	105.80
33	BA	2454	A	C8-N9-C4	5.77	108.11	105.80
33	BA	2507	A	N3-C4-N9	5.77	132.02	127.40
33	BA	2601	A	C4-C5-C6	5.77	119.89	117.00
33	BA	2777	A	C4-C5-C6	5.77	119.88	117.00
1	AA	1470	A	C8-N9-C4	5.77	108.11	105.80
33	BA	302	A	N9-C4-C5	5.77	108.11	105.80
33	BA	307	A	C8-N9-C4	5.77	108.11	105.80
33	BA	830	A	N3-C4-N9	5.77	132.01	127.40
33	BA	1325	A	C4-C5-C6	5.77	119.88	117.00
1	AA	452	A	N3-C4-N9	5.77	132.01	127.40
1	AA	1470	A	N3-C4-N9	5.77	132.01	127.40
33	BA	1025	A	N3-C4-N9	5.77	132.01	127.40
33	BA	1477	A	C8-N9-C4	5.77	108.11	105.80
33	BA	1961	A	C8-N9-C4	5.77	108.11	105.80
33	BA	2340	A	C8-N9-C4	5.77	108.11	105.80
33	BA	2594	A	C8-N9-C4	5.77	108.11	105.80
1	AA	258	A	C8-N9-C4	5.76	108.11	105.80
1	AA	278	A	C8-N9-C4	5.76	108.11	105.80
1	AA	651	A	N3-C4-N9	5.76	132.01	127.40
1	AA	1102	A	N3-C4-N9	5.76	132.01	127.40
33	BA	110	A	C8-N9-C4	5.76	108.11	105.80
33	BA	133	A	C8-N9-C4	5.76	108.11	105.80
33	BA	1555	A	C8-N9-C4	5.76	108.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1812	A	C4-C5-C6	5.76	119.88	117.00
33	BA	2908	A	C8-N9-C4	5.76	108.11	105.80
34	BB	64	A	C8-N9-C4	5.76	108.11	105.80
1	AA	211	A	C4-C5-C6	5.76	119.88	117.00
1	AA	506	A	N3-C4-N9	5.76	132.01	127.40
1	AA	582	A	C4-C5-C6	5.76	119.88	117.00
1	AA	910	A	C8-N9-C4	5.76	108.11	105.80
1	AA	1541	A	N3-C4-N9	5.76	132.01	127.40
33	BA	888	A	N3-C4-N9	5.76	132.01	127.40
33	BA	1047	A	C8-N9-C4	5.76	108.11	105.80
33	BA	2030	A	N3-C4-N9	5.76	132.01	127.40
33	BA	2307	A	N3-C4-N9	5.76	132.01	127.40
33	BA	2357	A	N9-C4-C5	5.76	108.11	105.80
33	BA	2447	A	C4-C5-N7	-5.76	107.82	110.70
33	BA	2482	A	N3-C4-N9	5.76	132.01	127.40
1	AA	62	A	C8-N9-C4	5.76	108.10	105.80
1	AA	386	A	N3-C4-N9	5.76	132.01	127.40
1	AA	771	A	C8-N9-C4	5.76	108.10	105.80
1	AA	825	A	N3-C4-N9	5.76	132.01	127.40
33	BA	314	A	C4-C5-C6	5.76	119.88	117.00
33	BA	337	A	C8-N9-C4	5.76	108.10	105.80
33	BA	584	A	N3-C4-N9	5.76	132.01	127.40
33	BA	1818	A	N3-C4-N9	5.76	132.01	127.40
33	BA	2276	A	C8-N9-C4	5.76	108.10	105.80
1	AA	1205	A	C4-C5-C6	5.76	119.88	117.00
33	BA	345	A	N3-C4-N9	5.76	132.01	127.40
33	BA	582	A	N3-C4-N9	5.76	132.01	127.40
33	BA	917	A	N3-C4-N9	5.76	132.01	127.40
33	BA	999	A	C8-N9-C4	5.76	108.10	105.80
33	BA	1727	A	C8-N9-C4	5.76	108.10	105.80
33	BA	2819	A	C4-C5-C6	5.76	119.88	117.00
34	BB	114	A	C8-N9-C4	5.76	108.10	105.80
1	AA	10	A	C4-C5-N7	-5.76	107.82	110.70
1	AA	202	A	N3-C4-N9	5.76	132.01	127.40
1	AA	210	A	N3-C4-N9	5.76	132.00	127.40
1	AA	228	A	N3-C4-N9	5.76	132.00	127.40
1	AA	423	A	C8-N9-C4	5.76	108.10	105.80
1	AA	651	A	C8-N9-C4	5.76	108.10	105.80
1	AA	737	A	C4-C5-N7	-5.76	107.82	110.70
1	AA	831	A	N3-C4-N9	5.76	132.00	127.40
1	AA	1257	A	C8-N9-C4	5.76	108.10	105.80
1	AA	1470	A	C4-C5-C6	5.76	119.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1528	A	C8-N9-C4	5.76	108.10	105.80
33	BA	64	A	C4-C5-C6	5.76	119.88	117.00
33	BA	504	A	C8-N9-C4	5.76	108.10	105.80
33	BA	1061	A	C4-C5-C6	5.76	119.88	117.00
33	BA	1417	A	C4-C5-N7	-5.76	107.82	110.70
33	BA	2052	A	C8-N9-C4	5.76	108.10	105.80
1	AA	31	A	C4-C5-C6	5.75	119.88	117.00
1	AA	1386	A	N3-C4-N9	5.75	132.00	127.40
33	BA	1008	A	C8-N9-C4	5.75	108.10	105.80
33	BA	1517	A	N3-C4-N9	5.75	132.00	127.40
33	BA	2134	A	C4-C5-C6	5.75	119.88	117.00
1	AA	117	A	C8-N9-C4	5.75	108.10	105.80
1	AA	816	A	N3-C4-N9	5.75	132.00	127.40
1	AA	1222	A	C8-N9-C4	5.75	108.10	105.80
33	BA	991	A	C4-C5-C6	5.75	119.88	117.00
33	BA	2782	A	C4-C5-N7	-5.75	107.82	110.70
1	AA	1328	A	C8-N9-C4	5.75	108.10	105.80
1	AA	1512	A	C8-N9-C4	5.75	108.10	105.80
33	BA	247	A	N3-C4-N9	5.75	132.00	127.40
33	BA	342	A	N3-C4-N9	5.75	132.00	127.40
33	BA	572	A	C8-N9-C4	5.75	108.10	105.80
33	BA	2593	A	N3-C4-N9	5.75	132.00	127.40
1	AA	1348	A	C8-N9-C4	5.75	108.10	105.80
33	BA	1021	A	N3-C4-N9	5.75	132.00	127.40
33	BA	1601	A	C4-C5-C6	5.75	119.88	117.00
33	BA	2254	A	C8-N9-C4	5.75	108.10	105.80
33	BA	2670	A	N9-C4-C5	5.75	108.10	105.80
34	BB	102	A	N9-C4-C5	5.75	108.10	105.80
1	AA	506	A	N9-C4-C5	5.75	108.10	105.80
1	AA	883	A	C8-N9-C4	5.75	108.10	105.80
1	AA	1298	A	C8-N9-C4	5.75	108.10	105.80
33	BA	618	A	C4-C5-C6	5.75	119.87	117.00
33	BA	952	A	C8-N9-C4	5.75	108.10	105.80
33	BA	1130	A	N3-C4-N9	5.75	132.00	127.40
33	BA	1615	A	C8-N9-C4	5.75	108.10	105.80
33	BA	2163	A	C8-N9-C4	5.75	108.10	105.80
33	BA	2398	A	C4-C5-N7	-5.75	107.83	110.70
1	AA	206	A	N3-C4-N9	5.75	132.00	127.40
1	AA	382	A	C8-N9-C4	5.75	108.10	105.80
33	BA	244	A	C8-N9-C4	5.75	108.10	105.80
33	BA	476	A	N9-C4-C5	5.75	108.10	105.80
33	BA	2779	A	N9-C4-C5	5.75	108.10	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	542	A	C8-N9-C4	5.75	108.10	105.80
33	BA	126	A	C4-C5-C6	5.75	119.87	117.00
33	BA	374	A	C4-C5-N7	-5.75	107.83	110.70
33	BA	2088	A	N3-C4-N9	5.75	132.00	127.40
33	BA	2455	A	N3-C4-N9	5.75	132.00	127.40
1	AA	190	A	C8-N9-C4	5.74	108.10	105.80
1	AA	202	A	C8-N9-C4	5.74	108.10	105.80
1	AA	344	A	C8-N9-C4	5.74	108.10	105.80
1	AA	541	A	N3-C4-N9	5.74	132.00	127.40
1	AA	791	A	N3-C4-N9	5.74	131.99	127.40
1	AA	1048	A	N3-C4-N9	5.74	132.00	127.40
1	AA	1254	A	C4-C5-C6	5.74	119.87	117.00
1	AA	1434	A	C4-C5-C6	5.74	119.87	117.00
1	AA	1513	A	C8-N9-C4	5.74	108.10	105.80
33	BA	325	A	C8-N9-C4	5.74	108.10	105.80
33	BA	1046	A	C4-C5-C6	5.74	119.87	117.00
33	BA	1277	A	C8-N9-C4	5.74	108.10	105.80
33	BA	1461	A	C8-N9-C4	5.74	108.10	105.80
33	BA	2542	A	C8-N9-C4	5.74	108.10	105.80
1	AA	53	A	C8-N9-C4	5.74	108.10	105.80
1	AA	159	A	C4-C5-C6	5.74	119.87	117.00
1	AA	456	A	N3-C4-N9	5.74	131.99	127.40
1	AA	542	A	N3-C4-N9	5.74	131.99	127.40
1	AA	1541	A	C8-N9-C4	5.74	108.10	105.80
33	BA	199	A	N3-C4-N9	5.74	131.99	127.40
33	BA	840	A	C5-C6-N1	5.74	120.57	117.70
33	BA	1056	A	N3-C4-N9	5.74	131.99	127.40
33	BA	1269	A	C8-N9-C4	5.74	108.10	105.80
1	AA	1236	A	N9-C4-C5	5.74	108.10	105.80
33	BA	622	A	N3-C4-N9	5.74	131.99	127.40
33	BA	658	A	N3-C4-N9	5.74	131.99	127.40
33	BA	765	A	C4-C5-N7	-5.74	107.83	110.70
33	BA	1284	A	C8-N9-C4	5.74	108.10	105.80
1	AA	170	A	C4-C5-N7	-5.74	107.83	110.70
1	AA	504	A	C8-N9-C4	5.74	108.09	105.80
1	AA	618	A	C8-N9-C4	5.74	108.10	105.80
1	AA	1417	A	N3-C4-N9	5.74	131.99	127.40
1	AA	1443	A	N9-C4-C5	5.74	108.09	105.80
33	BA	322	A	N3-C4-N9	5.74	131.99	127.40
33	BA	448	A	C4-C5-C6	5.74	119.87	117.00
33	BA	702	A	N3-C4-N9	5.74	131.99	127.40
33	BA	1046	A	C4-C5-N7	-5.74	107.83	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1115	A	N3-C4-N9	5.74	131.99	127.40
33	BA	1116	A	C8-N9-C4	5.74	108.09	105.80
33	BA	1326	A	C8-N9-C4	5.74	108.10	105.80
33	BA	1517	A	C4-C5-C6	5.74	119.87	117.00
33	BA	1654	A	N3-C4-N9	5.74	131.99	127.40
33	BA	1672	A	C8-N9-C4	5.74	108.09	105.80
33	BA	2155	A	N3-C4-N9	5.74	131.99	127.40
33	BA	2330	A	C4-C5-N7	-5.74	107.83	110.70
1	AA	1017	A	N3-C4-N9	5.74	131.99	127.40
1	AA	1092	A	C8-N9-C4	5.74	108.09	105.80
33	BA	274	A	N3-C4-N9	5.74	131.99	127.40
33	BA	448	A	C8-N9-C4	5.74	108.09	105.80
33	BA	1061	A	C8-N9-C4	5.74	108.09	105.80
33	BA	1499	A	N3-C4-N9	5.74	131.99	127.40
33	BA	1679	A	N3-C4-N9	5.74	131.99	127.40
33	BA	1797	A	N3-C4-N9	5.74	131.99	127.40
33	BA	1905	A	C4-C5-N7	-5.74	107.83	110.70
1	AA	544	A	C8-N9-C4	5.74	108.09	105.80
1	AA	679	A	C8-N9-C4	5.74	108.09	105.80
1	AA	1405	A	C8-N9-C4	5.74	108.09	105.80
33	BA	268	A	N3-C4-N9	5.74	131.99	127.40
33	BA	302	A	C4-C5-N7	-5.74	107.83	110.70
33	BA	494	A	N9-C4-C5	5.74	108.09	105.80
33	BA	740	A	N3-C4-N9	5.74	131.99	127.40
33	BA	1084	A	C8-N9-C4	5.74	108.09	105.80
33	BA	1791	A	N3-C4-N9	5.74	131.99	127.40
1	AA	1512	A	C4-C5-C6	5.73	119.87	117.00
33	BA	154	A	C4-C5-C6	5.73	119.87	117.00
33	BA	154	A	N3-C4-N9	5.73	131.99	127.40
33	BA	1947	A	C8-N9-C4	5.73	108.09	105.80
33	BA	2782	A	N3-C4-N9	5.73	131.99	127.40
34	BB	17	A	C8-N9-C4	5.73	108.09	105.80
1	AA	10	A	C4-C5-C6	5.73	119.87	117.00
1	AA	209	A	C4-C5-C6	5.73	119.87	117.00
1	AA	266	A	C8-N9-C4	5.73	108.09	105.80
1	AA	738	A	N3-C4-N9	5.73	131.99	127.40
1	AA	1503	A	N3-C4-N9	5.73	131.99	127.40
33	BA	219	A	C8-N9-C4	5.73	108.09	105.80
33	BA	268	A	N9-C4-C5	5.73	108.09	105.80
33	BA	389	A	N3-C4-N9	5.73	131.99	127.40
33	BA	1157	A	C4-C5-C6	5.73	119.87	117.00
33	BA	1815	A	N3-C4-N9	5.73	131.99	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2170	A	C8-N9-C4	5.73	108.09	105.80
33	BA	2191	A	N3-C4-N9	5.73	131.99	127.40
33	BA	2364	A	C4-C5-N7	-5.73	107.83	110.70
33	BA	2767	A	N3-C4-N9	5.73	131.99	127.40
1	AA	57	A	C8-N9-C4	5.73	108.09	105.80
1	AA	232	A	C4-C5-N7	-5.73	107.83	110.70
1	AA	266	A	C4-C5-N7	-5.73	107.83	110.70
33	BA	1202	A	N3-C4-N9	5.73	131.98	127.40
33	BA	2778	A	N3-C4-N9	5.73	131.98	127.40
33	BA	2793	A	N9-C4-C5	5.73	108.09	105.80
1	AA	556	A	C4-C5-N7	-5.73	107.83	110.70
33	BA	1194	A	C8-N9-C4	5.73	108.09	105.80
33	BA	1201	A	C4-C5-N7	-5.73	107.83	110.70
33	BA	2658	A	C8-N9-C4	5.73	108.09	105.80
1	AA	203	A	N3-C4-N9	5.73	131.98	127.40
1	AA	306	A	N3-C4-N9	5.73	131.98	127.40
1	AA	777	A	N3-C4-N9	5.73	131.98	127.40
1	AA	837	A	N3-C4-N9	5.73	131.98	127.40
1	AA	899	A	C4-C5-N7	-5.73	107.84	110.70
33	BA	202	A	C8-N9-C4	5.73	108.09	105.80
33	BA	1084	A	N3-C4-N9	5.73	131.98	127.40
33	BA	2315	A	C4-C5-C6	5.73	119.86	117.00
33	BA	2734	A	C8-N9-C4	5.73	108.09	105.80
1	AA	204	A	C8-N9-C4	5.73	108.09	105.80
33	BA	2357	A	N3-C4-N9	5.73	131.98	127.40
1	AA	159	A	N3-C4-N9	5.72	131.98	127.40
1	AA	581	A	N3-C4-N9	5.72	131.98	127.40
1	AA	837	A	C8-N9-C4	5.72	108.09	105.80
21	AX	58	A	C8-N9-C4	5.72	108.09	105.80
33	BA	84	A	C8-N9-C4	5.72	108.09	105.80
33	BA	389	A	C8-N9-C4	5.72	108.09	105.80
33	BA	752	A	C8-N9-C4	5.72	108.09	105.80
33	BA	1161	A	C8-N9-C4	5.72	108.09	105.80
33	BA	1585	A	C8-N9-C4	5.72	108.09	105.80
33	BA	2405	A	N3-C4-N9	5.72	131.98	127.40
1	AA	129	A	C8-N9-C4	5.72	108.09	105.80
1	AA	568	A	C4-C5-C6	5.72	119.86	117.00
1	AA	988	A	C8-N9-C4	5.72	108.09	105.80
1	AA	1358	A	C8-N9-C4	5.72	108.09	105.80
33	BA	501	A	C8-N9-C4	5.72	108.09	105.80
33	BA	910	A	C8-N9-C4	5.72	108.09	105.80
33	BA	2059	A	C8-N9-C4	5.72	108.09	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2200	A	C8-N9-C4	5.72	108.09	105.80
33	BA	2262	A	N9-C4-C5	5.72	108.09	105.80
33	BA	2907	A	C8-N9-C4	5.72	108.09	105.80
1	AA	228	A	C8-N9-C4	5.72	108.09	105.80
1	AA	582	A	N3-C4-N9	5.72	131.98	127.40
33	BA	646	A	C8-N9-C4	5.72	108.09	105.80
33	BA	999	A	C4-C5-C6	5.72	119.86	117.00
1	AA	1245	A	C8-N9-C4	5.72	108.09	105.80
33	BA	210	A	N3-C4-N9	5.72	131.98	127.40
33	BA	584	A	C4-C5-C6	5.72	119.86	117.00
33	BA	702	A	C4-C5-C6	5.72	119.86	117.00
33	BA	1119	A	C4-C5-C6	5.72	119.86	117.00
33	BA	1123	A	C8-N9-C4	5.72	108.09	105.80
33	BA	2256	A	C8-N9-C4	5.72	108.09	105.80
33	BA	2364	A	N3-C4-N9	5.72	131.97	127.40
34	BB	18	A	N9-C4-C5	5.72	108.09	105.80
1	AA	31	A	C8-N9-C4	5.72	108.09	105.80
1	AA	491	A	C8-N9-C4	5.72	108.09	105.80
1	AA	1443	A	C4-C5-N7	-5.72	107.84	110.70
33	BA	821	A	N3-C4-N9	5.72	131.97	127.40
33	BA	894	A	N9-C4-C5	5.72	108.09	105.80
33	BA	2507	A	C8-N9-C4	5.72	108.09	105.80
1	AA	189	A	C4-C5-N7	-5.72	107.84	110.70
1	AA	452	A	N9-C4-C5	5.72	108.09	105.80
1	AA	519	A	N3-C4-N9	5.72	131.97	127.40
1	AA	762	A	C8-N9-C4	5.72	108.09	105.80
1	AA	1358	A	N3-C4-N9	5.72	131.97	127.40
33	BA	1456	A	N3-C4-N9	5.72	131.97	127.40
33	BA	1713	A	N3-C4-N9	5.72	131.97	127.40
33	BA	1809	A	N3-C4-N9	5.72	131.97	127.40
33	BA	1948	A	C4-C5-C6	5.72	119.86	117.00
33	BA	2480	A	C4-C5-C6	5.72	119.86	117.00
33	BA	2480	A	N3-C4-N9	5.72	131.97	127.40
1	AA	148	A	C4-C5-C6	5.71	119.86	117.00
1	AA	776	A	C8-N9-C4	5.71	108.09	105.80
1	AA	1006	A	C8-N9-C4	5.71	108.09	105.80
1	AA	1166	A	C8-N9-C4	5.71	108.09	105.80
33	BA	1473	A	C4-C5-N7	-5.71	107.84	110.70
33	BA	1809	A	C8-N9-C4	5.71	108.09	105.80
33	BA	2091	A	N9-C4-C5	5.71	108.08	105.80
33	BA	2295	A	N9-C4-C5	5.71	108.09	105.80
33	BA	2479	A	N3-C4-N9	5.71	131.97	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2500	A	C8-N9-C4	5.71	108.08	105.80
33	BA	185	A	C5-C6-N1	5.71	120.56	117.70
1	AA	456	A	C8-N9-C4	5.71	108.08	105.80
1	AA	1022	A	C8-N9-C4	5.71	108.08	105.80
1	AA	1419	A	N3-C4-N9	5.71	131.97	127.40
33	BA	355	A	N3-C4-N9	5.71	131.97	127.40
33	BA	369	A	C8-N9-C4	5.71	108.08	105.80
33	BA	619	A	C4-C5-C6	5.71	119.86	117.00
33	BA	723	A	N9-C4-C5	5.71	108.08	105.80
33	BA	965	A	C4-C5-C6	5.71	119.86	117.00
33	BA	1161	A	N3-C4-N9	5.71	131.97	127.40
33	BA	1244	A	C4-C5-C6	5.71	119.86	117.00
33	BA	1339	A	N3-C4-N9	5.71	131.97	127.40
33	BA	1404	A	C8-N9-C4	5.71	108.08	105.80
33	BA	1929	A	N3-C4-N9	5.71	131.97	127.40
33	BA	2080	A	C8-N9-C4	5.71	108.08	105.80
33	BA	2227	A	C8-N9-C4	5.71	108.08	105.80
33	BA	2673	A	C8-N9-C4	5.71	108.08	105.80
34	BB	39	A	C8-N9-C4	5.71	108.08	105.80
34	BB	76	A	C8-N9-C4	5.71	108.08	105.80
34	BB	97	A	C8-N9-C4	5.71	108.08	105.80
1	AA	671	A	C8-N9-C4	5.71	108.08	105.80
1	AA	704	A	C8-N9-C4	5.71	108.08	105.80
1	AA	837	A	C4-C5-C6	5.71	119.86	117.00
1	AA	1349	A	C8-N9-C4	5.71	108.08	105.80
33	BA	274	A	C8-N9-C4	5.71	108.08	105.80
33	BA	1606	A	C8-N9-C4	5.71	108.08	105.80
1	AA	189	A	N9-C4-C5	5.71	108.08	105.80
1	AA	501	A	N3-C4-N9	5.71	131.97	127.40
1	AA	690	A	N3-C4-N9	5.71	131.97	127.40
1	AA	1451	A	C8-N9-C4	5.71	108.08	105.80
33	BA	202	A	N3-C4-N9	5.71	131.97	127.40
33	BA	224	A	C8-N9-C4	5.71	108.08	105.80
33	BA	1061	A	C4-C5-N7	-5.71	107.85	110.70
33	BA	1141	A	N3-C4-N9	5.71	131.97	127.40
33	BA	1142	A	C8-N9-C4	5.71	108.08	105.80
33	BA	1157	A	N3-C4-N9	5.71	131.97	127.40
33	BA	1412	A	N3-C4-N9	5.71	131.97	127.40
1	AA	31	A	N3-C4-N9	5.71	131.97	127.40
1	AA	870	A	N3-C4-N9	5.71	131.97	127.40
1	AA	1355	A	C4-C5-N7	-5.71	107.85	110.70
33	BA	1157	A	N9-C4-C5	5.71	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1686	A	C4-C5-N7	-5.71	107.85	110.70
33	BA	1942	A	C8-N9-C4	5.71	108.08	105.80
33	BA	1957	A	N3-C4-N9	5.71	131.97	127.40
33	BA	2315	A	N3-C4-N9	5.71	131.97	127.40
34	BB	18	A	C4-C5-N7	-5.71	107.85	110.70
1	AA	463	A	C8-N9-C4	5.71	108.08	105.80
1	AA	924	A	N3-C4-N9	5.71	131.96	127.40
33	BA	1375	A	C8-N9-C4	5.71	108.08	105.80
33	BA	2049	A	N9-C4-C5	5.71	108.08	105.80
33	BA	2362	A	N3-C4-N9	5.71	131.96	127.40
1	AA	419	A	C4-C5-N7	-5.70	107.85	110.70
1	AA	737	A	C4-C5-C6	5.70	119.85	117.00
1	AA	1254	A	C8-N9-C4	5.70	108.08	105.80
1	AA	1254	A	N3-C4-N9	5.70	131.96	127.40
1	AA	1271	A	C8-N9-C4	5.70	108.08	105.80
1	AA	1289	A	N3-C4-N9	5.70	131.96	127.40
1	AA	1296	A	C8-N9-C4	5.70	108.08	105.80
1	AA	1320	A	N9-C4-C5	5.70	108.08	105.80
1	AA	1422	A	C4-C5-C6	5.70	119.85	117.00
1	AA	1529	A	C8-N9-C4	5.70	108.08	105.80
33	BA	49	A	C4-C5-C6	5.70	119.85	117.00
33	BA	260	A	C8-N9-C4	5.70	108.08	105.80
33	BA	314	A	N3-C4-N9	5.70	131.96	127.40
33	BA	418	A	C8-N9-C4	5.70	108.08	105.80
33	BA	501	A	C4-C5-C6	5.70	119.85	117.00
33	BA	847	A	C4-C5-N7	-5.70	107.85	110.70
33	BA	1517	A	C8-N9-C4	5.70	108.08	105.80
33	BA	1966	A	N3-C4-N9	5.70	131.96	127.40
33	BA	2141	A	N3-C4-N9	5.70	131.96	127.40
33	BA	2296	A	N3-C4-N9	5.70	131.96	127.40
33	BA	2338	A	C8-N9-C4	5.70	108.08	105.80
34	BB	37	A	N3-C4-N9	5.70	131.96	127.40
1	AA	329	A	N3-C4-N9	5.70	131.96	127.40
1	AA	974	A	C8-N9-C4	5.70	108.08	105.80
33	BA	178	A	N3-C4-N9	5.70	131.96	127.40
33	BA	236	A	C8-N9-C4	5.70	108.08	105.80
33	BA	683	A	N9-C4-C5	5.70	108.08	105.80
33	BA	1224	A	C8-N9-C4	5.70	108.08	105.80
33	BA	2398	A	N9-C4-C5	5.70	108.08	105.80
33	BA	2463	A	N9-C4-C5	5.70	108.08	105.80
1	AA	195	A	N9-C4-C5	5.70	108.08	105.80
1	AA	240	A	C8-N9-C4	5.70	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	452	A	C4-C5-N7	-5.70	107.85	110.70
1	AA	477	A	C4-C5-C6	5.70	119.85	117.00
1	AA	569	A	C8-N9-C4	5.70	108.08	105.80
1	AA	777	A	C8-N9-C4	5.70	108.08	105.80
33	BA	117	A	N9-C4-C5	5.70	108.08	105.80
33	BA	1019	A	N9-C4-C5	5.70	108.08	105.80
33	BA	1347	A	C4-C5-C6	5.70	119.85	117.00
1	AA	323	A	N3-C4-N9	5.70	131.96	127.40
1	AA	367	A	N9-C4-C5	5.70	108.08	105.80
1	AA	974	A	N3-C4-N9	5.70	131.96	127.40
1	AA	1488	A	C4-C5-N7	-5.70	107.85	110.70
33	BA	459	A	C8-N9-C4	5.70	108.08	105.80
33	BA	999	A	N3-C4-N9	5.70	131.96	127.40
33	BA	1965	A	N3-C4-N9	5.70	131.96	127.40
1	AA	178	A	C8-N9-C4	5.70	108.08	105.80
1	AA	281	A	C8-N9-C4	5.70	108.08	105.80
33	BA	64	A	N3-C4-N9	5.70	131.96	127.40
33	BA	1533	A	C8-N9-C4	5.70	108.08	105.80
33	BA	2908	A	N3-C4-N9	5.70	131.96	127.40
1	AA	10	A	N3-C4-N9	5.70	131.96	127.40
1	AA	189	A	C8-N9-C4	5.70	108.08	105.80
1	AA	367	A	C4-C5-N7	-5.70	107.85	110.70
1	AA	925	A	N3-C4-N9	5.70	131.96	127.40
1	AA	1407	A	C4-C5-C6	5.70	119.85	117.00
33	BA	200	A	C8-N9-C4	5.70	108.08	105.80
33	BA	904	A	N3-C4-N9	5.70	131.96	127.40
33	BA	1601	A	N9-C4-C5	5.70	108.08	105.80
33	BA	1743	A	C8-N9-C4	5.70	108.08	105.80
33	BA	2119	A	C8-N9-C4	5.70	108.08	105.80
33	BA	2487	U	C2'-C3'-O3'	-5.70	96.97	109.50
33	BA	2854	A	C8-N9-C4	5.70	108.08	105.80
1	AA	232	A	C4-C5-C6	5.69	119.85	117.00
1	AA	419	A	C4-C5-C6	5.69	119.85	117.00
1	AA	929	A	N9-C4-C5	5.69	108.08	105.80
21	AX	37	A	N7-C8-N9	-5.69	110.95	113.80
33	BA	229	A	C8-N9-C4	5.69	108.08	105.80
33	BA	1802	A	C8-N9-C4	5.69	108.08	105.80
33	BA	2148	A	C8-N9-C4	5.69	108.08	105.80
33	BA	2295	A	C4-C5-C6	5.69	119.85	117.00
1	AA	203	A	C8-N9-C4	5.69	108.08	105.80
1	AA	232	A	N9-C4-C5	5.69	108.08	105.80
1	AA	508	A	C8-N9-C4	5.69	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	611	A	C8-N9-C4	5.69	108.08	105.80
1	AA	1247	A	C4-C5-N7	-5.69	107.85	110.70
33	BA	333	A	C8-N9-C4	5.69	108.08	105.80
33	BA	342	A	C4-C5-C6	5.69	119.85	117.00
33	BA	781	A	C8-N9-C4	5.69	108.08	105.80
33	BA	868	A	C8-N9-C4	5.69	108.08	105.80
33	BA	1123	A	N3-C4-N9	5.69	131.95	127.40
33	BA	1287	A	N3-C4-N9	5.69	131.95	127.40
33	BA	1913	A	C8-N9-C4	5.69	108.08	105.80
1	AA	438	A	N3-C4-N9	5.69	131.95	127.40
1	AA	828	A	C8-N9-C4	5.69	108.08	105.80
33	BA	156	A	C8-N9-C4	5.69	108.08	105.80
33	BA	2398	A	C8-N9-C4	5.69	108.08	105.80
33	BA	2835	A	C8-N9-C4	5.69	108.08	105.80
34	BB	17	A	C4-C5-N7	-5.69	107.86	110.70
1	AA	838	A	C8-N9-C4	5.69	108.08	105.80
33	BA	723	A	C8-N9-C4	5.69	108.08	105.80
33	BA	888	A	C4-C5-N7	-5.69	107.86	110.70
33	BA	1179	A	C8-N9-C4	5.69	108.08	105.80
33	BA	1593	A	C8-N9-C4	5.69	108.08	105.80
33	BA	2463	A	N3-C4-N9	5.69	131.95	127.40
1	AA	208	A	N3-C4-N9	5.69	131.95	127.40
1	AA	664	A	C8-N9-C4	5.69	108.08	105.80
33	BA	376	A	C8-N9-C4	5.69	108.08	105.80
33	BA	957	A	C4-C5-N7	-5.69	107.86	110.70
33	BA	991	A	C8-N9-C4	5.69	108.08	105.80
33	BA	1583	A	C8-N9-C4	5.69	108.08	105.80
33	BA	2042	A	C8-N9-C4	5.69	108.08	105.80
33	BA	2071	A	N3-C4-N9	5.69	131.95	127.40
33	BA	2317	A	C8-N9-C4	5.69	108.08	105.80
33	BA	2618	A	N9-C4-C5	5.69	108.08	105.80
33	BA	2782	A	N9-C4-C5	5.69	108.08	105.80
1	AA	1488	A	N9-C4-C5	5.69	108.07	105.80
33	BA	732	A	C5-C6-N1	5.69	120.54	117.70
33	BA	821	A	C4-C5-C6	5.69	119.84	117.00
33	BA	1323	A	C8-N9-C4	5.69	108.07	105.80
33	BA	1357	A	C8-N9-C4	5.69	108.08	105.80
33	BA	1432	A	C8-N9-C4	5.69	108.07	105.80
33	BA	2298	A	C8-N9-C4	5.69	108.07	105.80
33	BA	2907	A	C4-C5-N7	-5.69	107.86	110.70
1	AA	18	A	N3-C4-N9	5.68	131.95	127.40
1	AA	178	A	C4-C5-N7	-5.68	107.86	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	456	A	C4-C5-N7	-5.68	107.86	110.70
1	AA	616	A	C8-N9-C4	5.68	108.07	105.80
1	AA	959	A	C4-C5-N7	-5.68	107.86	110.70
1	AA	1050	A	N9-C4-C5	5.68	108.07	105.80
33	BA	49	A	N9-C4-C5	5.68	108.07	105.80
33	BA	125	A	C4-C5-N7	-5.68	107.86	110.70
33	BA	476	A	C4-C5-N7	-5.68	107.86	110.70
33	BA	572	A	N3-C4-N9	5.68	131.95	127.40
33	BA	1266	A	N3-C4-N9	5.68	131.95	127.40
33	BA	1483	A	C8-N9-C4	5.68	108.07	105.80
33	BA	1532	A	C8-N9-C4	5.68	108.07	105.80
33	BA	2276	A	N3-C4-N9	5.68	131.95	127.40
33	BA	2835	A	N3-C4-N9	5.68	131.95	127.40
1	AA	1422	A	C8-N9-C4	5.68	108.07	105.80
1	AA	1517	A	C8-N9-C4	5.68	108.07	105.80
33	BA	1579	A	N9-C4-C5	5.68	108.07	105.80
33	BA	2071	A	C8-N9-C4	5.68	108.07	105.80
1	AA	496	A	C8-N9-C4	5.68	108.07	105.80
33	BA	2694	A	C8-N9-C4	5.68	108.07	105.80
1	AA	725	A	N3-C4-N9	5.68	131.94	127.40
33	BA	28	A	C4-C5-C6	5.68	119.84	117.00
33	BA	162	A	C4-C5-C6	5.68	119.84	117.00
33	BA	1020	A	C8-N9-C4	5.68	108.07	105.80
33	BA	1026	A	C8-N9-C4	5.68	108.07	105.80
33	BA	1061	A	N9-C4-C5	5.68	108.07	105.80
33	BA	1144	A	C8-N9-C4	5.68	108.07	105.80
33	BA	1406	A	C8-N9-C4	5.68	108.07	105.80
33	BA	2362	A	C4-C5-C6	5.68	119.84	117.00
1	AA	422	A	C8-N9-C4	5.68	108.07	105.80
1	AA	508	A	C4-C5-N7	-5.68	107.86	110.70
1	AA	738	A	C8-N9-C4	5.68	108.07	105.80
33	BA	388	A	C8-N9-C4	5.68	108.07	105.80
33	BA	1504	A	C8-N9-C4	5.68	108.07	105.80
33	BA	2417	A	C4-C5-N7	-5.68	107.86	110.70
33	BA	2805	A	C4-C5-N7	-5.68	107.86	110.70
1	AA	234	A	C8-N9-C4	5.68	108.07	105.80
1	AA	969	A	N3-C4-N9	5.68	131.94	127.40
1	AA	1205	A	C8-N9-C4	5.68	108.07	105.80
1	AA	1207	A	N3-C4-N9	5.68	131.94	127.40
1	AA	1270	A	C8-N9-C4	5.68	108.07	105.80
33	BA	418	A	C4-C5-C6	5.68	119.84	117.00
33	BA	1084	A	C4-C5-N7	-5.68	107.86	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1161	A	C4-C5-N7	-5.68	107.86	110.70
33	BA	1432	A	C4-C5-C6	5.68	119.84	117.00
33	BA	1442	A	C8-N9-C4	5.68	108.07	105.80
33	BA	2297	A	C8-N9-C4	5.68	108.07	105.80
33	BA	2315	A	C4-C5-N7	-5.68	107.86	110.70
33	BA	2398	A	C4-C5-C6	5.68	119.84	117.00
1	AA	178	A	N3-C4-N9	5.67	131.94	127.40
1	AA	419	A	N9-C4-C5	5.67	108.07	105.80
1	AA	757	A	C8-N9-C4	5.67	108.07	105.80
1	AA	925	A	C4-C5-C6	5.67	119.84	117.00
33	BA	6	A	C8-N9-C4	5.67	108.07	105.80
33	BA	139	A	C8-N9-C4	5.67	108.07	105.80
33	BA	183	A	C4-C5-N7	-5.67	107.86	110.70
33	BA	667	A	C4-C5-N7	-5.67	107.86	110.70
33	BA	957	A	N9-C4-C5	5.67	108.07	105.80
33	BA	1734	A	C8-N9-C4	5.67	108.07	105.80
33	BA	2477	A	C8-N9-C4	5.67	108.07	105.80
1	AA	148	A	N3-C4-N9	5.67	131.94	127.40
1	AA	1289	A	C8-N9-C4	5.67	108.07	105.80
1	AA	1479	A	C8-N9-C4	5.67	108.07	105.80
33	BA	2618	A	C4-C5-N7	-5.67	107.86	110.70
1	AA	522	A	C8-N9-C4	5.67	108.07	105.80
1	AA	768	A	C4-C5-N7	-5.67	107.86	110.70
1	AA	924	A	C4-C5-C6	5.67	119.83	117.00
1	AA	1207	A	C8-N9-C4	5.67	108.07	105.80
1	AA	1434	A	N3-C4-N9	5.67	131.94	127.40
1	AA	1442	A	C8-N9-C4	5.67	108.07	105.80
33	BA	1066	A	C8-N9-C4	5.67	108.07	105.80
33	BA	1119	A	N3-C4-N9	5.67	131.94	127.40
33	BA	1412	A	C8-N9-C4	5.67	108.07	105.80
33	BA	1540	A	C8-N9-C4	5.67	108.07	105.80
33	BA	1661	A	N7-C8-N9	-5.67	110.97	113.80
33	BA	2464	A	C4-C5-N7	-5.67	107.86	110.70
33	BA	179	A	C4-C5-N7	-5.67	107.86	110.70
33	BA	811	A	C4-C5-C6	5.67	119.83	117.00
33	BA	1845	A	C8-N9-C4	5.67	108.07	105.80
1	AA	296	A	C8-N9-C4	5.67	108.07	105.80
1	AA	440	A	C4-C5-N7	-5.67	107.86	110.70
1	AA	1417	A	C8-N9-C4	5.67	108.07	105.80
33	BA	530	A	C8-N9-C4	5.67	108.07	105.80
33	BA	622	A	N9-C4-C5	5.67	108.07	105.80
33	BA	758	A	C8-N9-C4	5.67	108.07	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1005	A	N9-C4-C5	5.67	108.07	105.80
33	BA	1776	A	C8-N9-C4	5.67	108.07	105.80
33	BA	2276	A	C4-C5-C6	5.67	119.83	117.00
1	AA	306	A	C8-N9-C4	5.67	108.07	105.80
1	AA	422	A	C4-C5-N7	-5.67	107.87	110.70
33	BA	322	A	C8-N9-C4	5.67	108.07	105.80
33	BA	354	A	C8-N9-C4	5.67	108.07	105.80
33	BA	2668	A	C8-N9-C4	5.67	108.07	105.80
1	AA	440	A	C8-N9-C4	5.67	108.07	105.80
1	AA	886	A	C8-N9-C4	5.67	108.07	105.80
1	AA	1252	A	C8-N9-C4	5.67	108.07	105.80
33	BA	1948	A	N3-C4-N9	5.67	131.93	127.40
1	AA	67	A	C8-N9-C4	5.66	108.06	105.80
33	BA	305	A	C8-N9-C4	5.66	108.06	105.80
33	BA	477	A	C4-C5-N7	-5.66	107.87	110.70
33	BA	1174	A	C8-N9-C4	5.66	108.07	105.80
33	BA	1175	A	N3-C4-N9	5.66	131.93	127.40
33	BA	1461	A	C4-C5-N7	-5.66	107.87	110.70
33	BA	1569	A	C8-N9-C4	5.66	108.06	105.80
33	BA	2295	A	N3-C4-N9	5.66	131.93	127.40
33	BA	2479	A	C8-N9-C4	5.66	108.06	105.80
33	BA	2482	A	C8-N9-C4	5.66	108.06	105.80
33	BA	2846	A	C8-N9-C4	5.66	108.07	105.80
1	AA	170	A	N3-C4-N9	5.66	131.93	127.40
33	BA	504	A	C4-C5-N7	-5.66	107.87	110.70
33	BA	575	A	N9-C4-C5	5.66	108.06	105.80
33	BA	1601	A	N3-C4-N9	5.66	131.93	127.40
33	BA	2767	A	C8-N9-C4	5.66	108.06	105.80
1	AA	415	A	C4-C5-C6	5.66	119.83	117.00
1	AA	422	A	N3-C4-N9	5.66	131.93	127.40
1	AA	969	A	N9-C4-C5	5.66	108.06	105.80
1	AA	978	A	N9-C4-C5	5.66	108.06	105.80
33	BA	140	A	C8-N9-C4	5.66	108.06	105.80
33	BA	166	A	N3-C4-N9	5.66	131.93	127.40
33	BA	786	A	C8-N9-C4	5.66	108.06	105.80
33	BA	1092	A	N3-C4-N9	5.66	131.93	127.40
33	BA	1189	A	N3-C4-N9	5.66	131.93	127.40
33	BA	2919	A	C8-N9-C4	5.66	108.06	105.80
34	BB	55	A	C8-N9-C4	5.66	108.06	105.80
1	AA	31	A	C4-C5-N7	-5.66	107.87	110.70
1	AA	34	A	C8-N9-C4	5.66	108.06	105.80
1	AA	371	A	C8-N9-C4	5.66	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	816	A	C8-N9-C4	5.66	108.06	105.80
1	AA	947	A	C8-N9-C4	5.66	108.06	105.80
33	BA	161	A	C4-C5-N7	-5.66	107.87	110.70
33	BA	162	A	N3-C4-N9	5.66	131.93	127.40
33	BA	677	A	C8-N9-C4	5.66	108.06	105.80
33	BA	1210	A	N9-C4-C5	5.66	108.06	105.80
33	BA	1287	A	C8-N9-C4	5.66	108.06	105.80
33	BA	1638	A	C8-N9-C4	5.66	108.06	105.80
33	BA	2595	A	C4-C5-C6	5.66	119.83	117.00
33	BA	2812	A	C8-N9-C4	5.66	108.06	105.80
33	BA	224	A	N3-C4-N9	5.66	131.93	127.40
33	BA	1483	A	C4-C5-N7	-5.66	107.87	110.70
33	BA	2262	A	C4-C5-C6	5.66	119.83	117.00
33	BA	2356	A	C8-N9-C4	5.66	108.06	105.80
1	AA	76	A	C8-N9-C4	5.66	108.06	105.80
1	AA	208	A	C4-C5-C6	5.66	119.83	117.00
1	AA	592	A	C8-N9-C4	5.66	108.06	105.80
1	AA	988	A	N9-C4-C5	5.66	108.06	105.80
33	BA	1325	A	N3-C4-N9	5.66	131.92	127.40
33	BA	2047	A	C8-N9-C4	5.66	108.06	105.80
33	BA	2307	A	C4-C5-N7	-5.66	107.87	110.70
33	BA	2375	A	N9-C4-C5	5.66	108.06	105.80
33	BA	2593	A	N9-C4-C5	5.66	108.06	105.80
33	BA	991	A	N3-C4-N9	5.65	131.92	127.40
33	BA	1254	A	C8-N9-C4	5.65	108.06	105.80
1	AA	357	A	C8-N9-C4	5.65	108.06	105.80
1	AA	569	A	N3-C4-N9	5.65	131.92	127.40
1	AA	923	A	N3-C4-N9	5.65	131.92	127.40
1	AA	1488	A	N3-C4-N9	5.65	131.92	127.40
33	BA	278	A	C4-C5-N7	-5.65	107.87	110.70
33	BA	575	A	C4-C5-N7	-5.65	107.87	110.70
33	BA	1042	A	C8-N9-C4	5.65	108.06	105.80
33	BA	1113	A	C8-N9-C4	5.65	108.06	105.80
33	BA	1654	A	C4-C5-N7	-5.65	107.87	110.70
33	BA	2152	A	C4-C5-N7	-5.65	107.87	110.70
33	BA	2686	A	C8-N9-C4	5.65	108.06	105.80
1	AA	405	A	C5-C6-N1	5.65	120.53	117.70
1	AA	1115	A	C8-N9-C4	5.65	108.06	105.80
1	AA	1284	A	C8-N9-C4	5.65	108.06	105.80
1	AA	1327	A	C8-N9-C4	5.65	108.06	105.80
33	BA	194	A	C8-N9-C4	5.65	108.06	105.80
33	BA	244	A	C4-C5-C6	5.65	119.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	345	A	C8-N9-C4	5.65	108.06	105.80
33	BA	690	A	C8-N9-C4	5.65	108.06	105.80
33	BA	717	A	C4-C5-N7	-5.65	107.88	110.70
33	BA	978	A	C8-N9-C4	5.65	108.06	105.80
33	BA	1210	A	C4-C5-N7	-5.65	107.88	110.70
33	BA	2505	A	C8-N9-C4	5.65	108.06	105.80
1	AA	389	A	C8-N9-C4	5.65	108.06	105.80
1	AA	929	A	N3-C4-N9	5.65	131.92	127.40
33	BA	1966	A	C8-N9-C4	5.65	108.06	105.80
1	AA	211	A	C8-N9-C4	5.65	108.06	105.80
1	AA	236	A	C8-N9-C4	5.65	108.06	105.80
1	AA	658	A	C8-N9-C4	5.65	108.06	105.80
1	AA	775	A	N3-C4-N9	5.65	131.92	127.40
1	AA	886	A	C4-C5-N7	-5.65	107.88	110.70
1	AA	1090	A	N3-C4-N9	5.65	131.92	127.40
33	BA	318	A	C8-N9-C4	5.65	108.06	105.80
33	BA	847	A	N9-C4-C5	5.65	108.06	105.80
33	BA	917	A	C8-N9-C4	5.65	108.06	105.80
33	BA	1405	A	C8-N9-C4	5.65	108.06	105.80
33	BA	1608	A	C8-N9-C4	5.65	108.06	105.80
33	BA	1930	A	C4-C5-C6	5.65	119.82	117.00
33	BA	2132	A	C8-N9-C4	5.65	108.06	105.80
33	BA	2683	A	C4-C5-C6	5.65	119.82	117.00
33	BA	2778	A	N9-C4-C5	5.65	108.06	105.80
33	BA	2908	A	C4-C5-C6	5.65	119.82	117.00
34	BB	17	A	N3-C4-N9	5.65	131.92	127.40
1	AA	254	A	C4-C5-N7	-5.65	107.88	110.70
33	BA	2787	A	C8-N9-C4	5.65	108.06	105.80
1	AA	321	A	N3-C4-N9	5.64	131.92	127.40
1	AA	321	A	N9-C4-C5	5.64	108.06	105.80
21	AX	21	A	C8-N9-C4	5.64	108.06	105.80
33	BA	210	A	C8-N9-C4	5.64	108.06	105.80
33	BA	551	A	C4-C5-N7	-5.64	107.88	110.70
33	BA	1914	A	C4-C5-C6	5.64	119.82	117.00
33	BA	2595	A	N9-C4-C5	5.64	108.06	105.80
33	BA	2777	A	N3-C4-N9	5.64	131.91	127.40
1	AA	713	A	N3-C4-N9	5.64	131.91	127.40
1	AA	928	A	C8-N9-C4	5.64	108.06	105.80
1	AA	1112	A	C8-N9-C4	5.64	108.06	105.80
33	BA	102	A	C8-N9-C4	5.64	108.06	105.80
33	BA	364	A	C8-N9-C4	5.64	108.06	105.80
33	BA	763	A	C8-N9-C4	5.64	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1233	A	C8-N9-C4	5.64	108.06	105.80
33	BA	1914	A	N3-C4-N9	5.64	131.91	127.40
33	BA	1941	A	C4-C5-N7	-5.64	107.88	110.70
33	BA	1982	A	C4-C5-C6	5.64	119.82	117.00
33	BA	2383	A	N3-C4-N9	5.64	131.91	127.40
33	BA	2804	A	N9-C4-C5	5.64	108.06	105.80
33	BA	1287	A	C4-C5-N7	-5.64	107.88	110.70
33	BA	2152	A	C8-N9-C4	5.64	108.06	105.80
1	AA	439	A	N3-C4-N9	5.64	131.91	127.40
33	BA	561	A	C8-N9-C4	5.64	108.06	105.80
33	BA	770	A	C8-N9-C4	5.64	108.06	105.80
33	BA	811	A	C4-C5-N7	-5.64	107.88	110.70
33	BA	991	A	C4-C5-N7	-5.64	107.88	110.70
33	BA	1025	A	C4-C5-N7	-5.64	107.88	110.70
33	BA	1029	A	N9-C4-C5	5.64	108.06	105.80
33	BA	1175	A	C8-N9-C4	5.64	108.06	105.80
33	BA	2375	A	C8-N9-C4	5.64	108.06	105.80
33	BA	2916	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	151	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	556	A	N9-C4-C5	5.64	108.06	105.80
1	AA	737	A	N3-C4-N9	5.64	131.91	127.40
1	AA	1383	A	C8-N9-C4	5.64	108.06	105.80
33	BA	429	A	C8-N9-C4	5.64	108.06	105.80
33	BA	935	A	N9-C4-C5	5.64	108.06	105.80
33	BA	1119	A	N9-C4-C5	5.64	108.06	105.80
1	AA	796	A	C4-C5-N7	-5.64	107.88	110.70
33	BA	553	A	C8-N9-C4	5.64	108.05	105.80
33	BA	658	A	N9-C4-C5	5.64	108.05	105.80
33	BA	683	A	N3-C4-N9	5.64	131.91	127.40
33	BA	1025	A	N9-C4-C5	5.64	108.05	105.80
33	BA	1392	A	C8-N9-C4	5.64	108.06	105.80
33	BA	1906	A	C8-N9-C4	5.64	108.05	105.80
33	BA	2191	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	985	A	N3-C4-N9	5.63	131.91	127.40
33	BA	225	A	C8-N9-C4	5.63	108.05	105.80
33	BA	507	A	C8-N9-C4	5.63	108.05	105.80
33	BA	717	A	C8-N9-C4	5.63	108.05	105.80
33	BA	1516	A	C8-N9-C4	5.63	108.05	105.80
33	BA	1746	A	C8-N9-C4	5.63	108.05	105.80
1	AA	28	A	N3-C4-N9	5.63	131.91	127.40
1	AA	139	A	C4-C5-N7	-5.63	107.88	110.70
1	AA	282	A	C8-N9-C4	5.63	108.05	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	422	A	N9-C4-C5	5.63	108.05	105.80
1	AA	642	U	C2-N1-C1'	5.63	124.46	117.70
1	AA	831	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1048	A	C8-N9-C4	5.63	108.05	105.80
33	BA	224	A	C4-C5-C6	5.63	119.82	117.00
33	BA	2912	A	C8-N9-C4	5.63	108.05	105.80
1	AA	404	A	C8-N9-C4	5.63	108.05	105.80
1	AA	801	A	C8-N9-C4	5.63	108.05	105.80
1	AA	816	A	C4-C5-N7	-5.63	107.89	110.70
33	BA	67	A	C8-N9-C4	5.63	108.05	105.80
33	BA	117	A	C4-C5-N7	-5.63	107.88	110.70
33	BA	273	A	C4-C5-N7	-5.63	107.88	110.70
33	BA	908	A	N9-C4-C5	5.63	108.05	105.80
33	BA	1815	A	C4-C5-N7	-5.63	107.88	110.70
33	BA	2837	A	C4-C5-N7	-5.63	107.88	110.70
34	BB	27	A	C8-N9-C4	5.63	108.05	105.80
1	AA	148	A	C4-C5-N7	-5.63	107.89	110.70
1	AA	401	A	N3-C4-N9	5.63	131.90	127.40
1	AA	879	A	N3-C4-N9	5.63	131.90	127.40
1	AA	1342	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1512	A	N3-C4-N9	5.63	131.90	127.40
33	BA	49	A	N3-C4-N9	5.63	131.90	127.40
33	BA	1258	A	C8-N9-C4	5.63	108.05	105.80
33	BA	1797	A	C4-C5-N7	-5.63	107.89	110.70
33	BA	2134	A	N3-C4-N9	5.63	131.90	127.40
33	BA	2819	A	N3-C4-N9	5.63	131.90	127.40
1	AA	266	A	N3-C4-N9	5.63	131.90	127.40
1	AA	477	A	C4-C5-N7	-5.63	107.89	110.70
1	AA	796	A	C8-N9-C4	5.63	108.05	105.80
1	AA	924	A	N9-C4-C5	5.63	108.05	105.80
33	BA	154	A	C8-N9-C4	5.63	108.05	105.80
33	BA	279	A	C4-C5-N7	-5.63	107.89	110.70
33	BA	519	A	C8-N9-C4	5.63	108.05	105.80
33	BA	637	A	C8-N9-C4	5.63	108.05	105.80
33	BA	970	A	C8-N9-C4	5.63	108.05	105.80
33	BA	1312	A	C8-N9-C4	5.63	108.05	105.80
33	BA	2405	A	N9-C4-C5	5.63	108.05	105.80
33	BA	2421	A	C8-N9-C4	5.63	108.05	105.80
1	AA	321	A	C4-C5-N7	-5.63	107.89	110.70
1	AA	631	A	C4-C5-N7	-5.63	107.89	110.70
1	AA	1254	A	C4-C5-N7	-5.63	107.89	110.70
33	BA	964	A	C8-N9-C4	5.63	108.05	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1157	A	C8-N9-C4	5.63	108.05	105.80
33	BA	1189	A	C4-C5-N7	-5.63	107.89	110.70
33	BA	1735	A	C8-N9-C4	5.63	108.05	105.80
33	BA	1809	A	C4-C5-N7	-5.63	107.89	110.70
33	BA	1948	A	C8-N9-C4	5.63	108.05	105.80
33	BA	2062	A	C8-N9-C4	5.63	108.05	105.80
1	AA	139	A	N9-C4-C5	5.62	108.05	105.80
1	AA	803	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	1419	A	C8-N9-C4	5.62	108.05	105.80
33	BA	652	A	C4-C5-N7	-5.62	107.89	110.70
33	BA	2369	A	C8-N9-C4	5.62	108.05	105.80
1	AA	519	A	N9-C4-C5	5.62	108.05	105.80
1	AA	1006	A	N3-C4-N9	5.62	131.90	127.40
21	AX	41	A	C8-N9-C4	5.62	108.05	105.80
33	BA	94	A	C8-N9-C4	5.62	108.05	105.80
33	BA	559	A	C8-N9-C4	5.62	108.05	105.80
33	BA	659	A	C8-N9-C4	5.62	108.05	105.80
33	BA	1918	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2000	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2302	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2618	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2754	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2889	A	C8-N9-C4	5.62	108.05	105.80
1	AA	875	A	C8-N9-C4	5.62	108.05	105.80
1	AA	1443	A	N3-C4-N9	5.62	131.90	127.40
1	AA	1490	A	C8-N9-C4	5.62	108.05	105.80
33	BA	140	A	C4-C5-N7	-5.62	107.89	110.70
33	BA	436	A	C8-N9-C4	5.62	108.05	105.80
33	BA	547	A	C8-N9-C4	5.62	108.05	105.80
33	BA	922	A	C4-C5-N7	-5.62	107.89	110.70
33	BA	1003	A	C4-C5-C6	5.62	119.81	117.00
33	BA	1072	A	C8-N9-C4	5.62	108.05	105.80
33	BA	1524	A	C8-N9-C4	5.62	108.05	105.80
33	BA	1575	A	C8-N9-C4	5.62	108.05	105.80
34	BB	17	A	N9-C4-C5	5.62	108.05	105.80
1	AA	28	A	C4-C5-C6	5.62	119.81	117.00
1	AA	522	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	1121	A	C8-N9-C4	5.62	108.05	105.80
33	BA	171	A	C8-N9-C4	5.62	108.05	105.80
33	BA	618	A	N3-C4-N9	5.62	131.90	127.40
33	BA	715	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2032	A	C8-N9-C4	5.62	108.05	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2498	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2700	A	C8-N9-C4	5.62	108.05	105.80
1	AA	159	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	367	A	N3-C4-N9	5.62	131.90	127.40
33	BA	870	A	C8-N9-C4	5.62	108.05	105.80
33	BA	888	A	C8-N9-C4	5.62	108.05	105.80
33	BA	1130	A	N9-C4-C5	5.62	108.05	105.80
33	BA	1157	A	C4-C5-N7	-5.62	107.89	110.70
33	BA	2007	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2117	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2241	A	C4-C5-C6	5.62	119.81	117.00
33	BA	2381	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2683	A	N3-C4-N9	5.62	131.90	127.40
33	BA	5	A	C8-N9-C4	5.62	108.05	105.80
33	BA	329	A	C8-N9-C4	5.62	108.05	105.80
33	BA	770	A	C4-C5-N7	-5.62	107.89	110.70
33	BA	1119	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2165	A	C8-N9-C4	5.62	108.05	105.80
1	AA	604	A	C8-N9-C4	5.62	108.05	105.80
1	AA	1213	A	N3-C4-N9	5.62	131.89	127.40
1	AA	1266	A	C8-N9-C4	5.62	108.05	105.80
1	AA	1407	A	N3-C4-N9	5.62	131.89	127.40
33	BA	44	A	N9-C4-C5	5.62	108.05	105.80
33	BA	118	A	C8-N9-C4	5.62	108.05	105.80
33	BA	258	A	C8-N9-C4	5.62	108.05	105.80
33	BA	476	A	N3-C4-N9	5.62	131.89	127.40
33	BA	486	A	C8-N9-C4	5.62	108.05	105.80
33	BA	762	A	C8-N9-C4	5.62	108.05	105.80
33	BA	829	A	C8-N9-C4	5.62	108.05	105.80
33	BA	1115	A	C4-C5-N7	-5.62	107.89	110.70
33	BA	1627	A	C8-N9-C4	5.62	108.05	105.80
33	BA	1812	A	N3-C4-N9	5.62	131.89	127.40
33	BA	2124	A	C8-N9-C4	5.62	108.05	105.80
33	BA	2662	A	C8-N9-C4	5.62	108.05	105.80
1	AA	18	A	C4-C5-C6	5.61	119.81	117.00
1	AA	173	A	C8-N9-C4	5.61	108.05	105.80
1	AA	232	A	C8-N9-C4	5.61	108.05	105.80
1	AA	364	A	C8-N9-C4	5.61	108.05	105.80
1	AA	658	A	C4-C5-N7	-5.61	107.89	110.70
1	AA	882	A	C8-N9-C4	5.61	108.05	105.80
1	AA	919	A	C4-C5-N7	-5.61	107.89	110.70
1	AA	1050	A	C4-C5-N7	-5.61	107.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	244	A	N3-C4-N9	5.61	131.89	127.40
33	BA	278	A	C8-N9-C4	5.61	108.05	105.80
33	BA	343	A	N9-C4-C5	5.61	108.05	105.80
33	BA	355	A	C8-N9-C4	5.61	108.05	105.80
33	BA	740	A	C4-C5-N7	-5.61	107.89	110.70
33	BA	782	A	C8-N9-C4	5.61	108.05	105.80
33	BA	2034	A	C8-N9-C4	5.61	108.05	105.80
33	BA	2790	A	C8-N9-C4	5.61	108.05	105.80
1	AA	1178	A	N9-C4-C5	5.61	108.05	105.80
33	BA	161	A	C4-C5-C6	5.61	119.81	117.00
33	BA	354	A	C4-C5-C6	5.61	119.81	117.00
33	BA	490	A	N3-C4-N9	5.61	131.89	127.40
33	BA	717	A	N3-C4-N9	5.61	131.89	127.40
33	BA	1202	A	C4-C5-N7	-5.61	107.89	110.70
33	BA	1432	A	N3-C4-N9	5.61	131.89	127.40
33	BA	2601	A	C4-C5-N7	-5.61	107.89	110.70
1	AA	57	A	C4-C5-N7	-5.61	107.89	110.70
1	AA	333	A	C8-N9-C4	5.61	108.04	105.80
1	AA	919	A	C8-N9-C4	5.61	108.05	105.80
1	AA	1102	A	C8-N9-C4	5.61	108.05	105.80
1	AA	1434	A	C4-C5-N7	-5.61	107.89	110.70
33	BA	166	A	C4-C5-N7	-5.61	107.89	110.70
33	BA	717	A	N9-C4-C5	5.61	108.04	105.80
33	BA	732	A	N9-C4-C5	5.61	108.04	105.80
33	BA	965	A	C8-N9-C4	5.61	108.04	105.80
33	BA	1197	A	C8-N9-C4	5.61	108.04	105.80
33	BA	1266	A	N9-C4-C5	5.61	108.04	105.80
33	BA	1434	A	C4-C5-C6	5.61	119.81	117.00
33	BA	2343	A	C8-N9-C4	5.61	108.05	105.80
33	BA	2902	A	C8-N9-C4	5.61	108.04	105.80
34	BB	39	A	C4-C5-N7	-5.61	107.89	110.70
1	AA	1111	A	C8-N9-C4	5.61	108.04	105.80
33	BA	1816	A	C8-N9-C4	5.61	108.04	105.80
33	BA	2362	A	C4-C5-N7	-5.61	107.89	110.70
33	BA	2398	A	N3-C4-N9	5.61	131.89	127.40
33	BA	2571	A	C8-N9-C4	5.61	108.04	105.80
33	BA	2722	A	C8-N9-C4	5.61	108.04	105.80
1	AA	150	A	C4-C5-N7	-5.61	107.90	110.70
1	AA	171	A	N3-C4-N9	5.61	131.88	127.40
1	AA	703	A	N3-C4-N9	5.61	131.89	127.40
1	AA	803	A	C8-N9-C4	5.61	108.04	105.80
1	AA	1259	A	C8-N9-C4	5.61	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1359	A	C8-N9-C4	5.61	108.04	105.80
33	BA	124	A	C8-N9-C4	5.61	108.04	105.80
33	BA	230	A	C8-N9-C4	5.61	108.04	105.80
33	BA	342	A	C8-N9-C4	5.61	108.04	105.80
33	BA	517	A	C8-N9-C4	5.61	108.04	105.80
33	BA	1097	A	N9-C4-C5	5.61	108.04	105.80
34	BB	102	A	C4-C5-N7	-5.61	107.90	110.70
1	AA	251	A	C4-C5-N7	-5.61	107.90	110.70
1	AA	485	A	C8-N9-C4	5.61	108.04	105.80
1	AA	501	A	C8-N9-C4	5.61	108.04	105.80
1	AA	775	A	N9-C4-C5	5.61	108.04	105.80
21	AX	23	A	C4-C5-C6	5.61	119.80	117.00
33	BA	125	A	C4-C5-C6	5.61	119.80	117.00
33	BA	302	A	N3-C4-N9	5.61	131.88	127.40
33	BA	692	A	C8-N9-C4	5.61	108.04	105.80
33	BA	991	A	N9-C4-C5	5.61	108.04	105.80
33	BA	1141	A	C8-N9-C4	5.61	108.04	105.80
33	BA	1325	A	C4-C5-N7	-5.61	107.90	110.70
33	BA	1423	A	C4-C5-N7	-5.61	107.90	110.70
33	BA	2087	A	C8-N9-C4	5.61	108.04	105.80
1	AA	170	A	C4-C5-C6	5.60	119.80	117.00
1	AA	401	A	C8-N9-C4	5.60	108.04	105.80
33	BA	475	A	C8-N9-C4	5.60	108.04	105.80
33	BA	828	A	C8-N9-C4	5.60	108.04	105.80
33	BA	1895	A	C4-C5-N7	-5.60	107.90	110.70
33	BA	1914	A	N9-C4-C5	5.60	108.04	105.80
1	AA	477	A	N9-C4-C5	5.60	108.04	105.80
1	AA	501	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	703	A	C4-C5-C6	5.60	119.80	117.00
1	AA	725	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	1028	A	C8-N9-C4	5.60	108.04	105.80
1	AA	1111	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	1178	A	C4-C5-N7	-5.60	107.90	110.70
33	BA	500	A	C8-N9-C4	5.60	108.04	105.80
33	BA	549	A	C8-N9-C4	5.60	108.04	105.80
33	BA	673	A	C8-N9-C4	5.60	108.04	105.80
33	BA	1313	A	C8-N9-C4	5.60	108.04	105.80
33	BA	1592	A	C8-N9-C4	5.60	108.04	105.80
33	BA	1784	A	N9-C4-C5	5.60	108.04	105.80
33	BA	1789	A	C8-N9-C4	5.60	108.04	105.80
33	BA	1797	A	N9-C4-C5	5.60	108.04	105.80
33	BA	1812	A	N9-C4-C5	5.60	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1914	A	C8-N9-C4	5.60	108.04	105.80
33	BA	2769	A	N9-C4-C5	5.60	108.04	105.80
34	BB	27	A	C4-C5-N7	-5.60	107.90	110.70
34	BB	43	A	C8-N9-C4	5.60	108.04	105.80
34	BB	44	A	C8-N9-C4	5.60	108.04	105.80
1	AA	1493	A	C8-N9-C4	5.60	108.04	105.80
1	AA	1502	A	C4-C5-N7	-5.60	107.90	110.70
33	BA	166	A	C8-N9-C4	5.60	108.04	105.80
33	BA	418	A	C4-C5-N7	-5.60	107.90	110.70
33	BA	1945	A	N9-C4-C5	5.60	108.04	105.80
33	BA	2296	A	N9-C4-C5	5.60	108.04	105.80
34	BB	102	A	N3-C4-N9	5.60	131.88	127.40
1	AA	208	A	N9-C4-C5	5.60	108.04	105.80
1	AA	529	A	C8-N9-C4	5.60	108.04	105.80
1	AA	1050	A	N3-C4-N9	5.60	131.88	127.40
1	AA	1077	A	N3-C4-N9	5.60	131.88	127.40
33	BA	67	A	N9-C4-C5	5.60	108.04	105.80
33	BA	1092	A	N9-C4-C5	5.60	108.04	105.80
33	BA	1316	A	C8-N9-C4	5.60	108.04	105.80
33	BA	1679	A	C8-N9-C4	5.60	108.04	105.80
33	BA	2043	A	C8-N9-C4	5.60	108.04	105.80
33	BA	2595	A	N3-C4-N9	5.60	131.88	127.40
33	BA	2804	A	N3-C4-N9	5.60	131.88	127.40
1	AA	329	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	928	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	956	A	C4-C5-N7	-5.60	107.90	110.70
33	BA	67	A	C4-C5-N7	-5.60	107.90	110.70
33	BA	652	A	C8-N9-C4	5.60	108.04	105.80
33	BA	1161	A	N9-C4-C5	5.60	108.04	105.80
33	BA	1253	A	C8-N9-C4	5.60	108.04	105.80
33	BA	125	A	N3-C4-N9	5.60	131.88	127.40
33	BA	224	A	N9-C4-C5	5.60	108.04	105.80
33	BA	888	A	N9-C4-C5	5.60	108.04	105.80
33	BA	1412	A	C4-C5-C6	5.60	119.80	117.00
33	BA	1814	A	C4-C5-N7	-5.60	107.90	110.70
34	BB	102	A	C4-C5-C6	5.60	119.80	117.00
1	AA	352	A	C8-N9-C4	5.59	108.04	105.80
33	BA	13	A	C8-N9-C4	5.59	108.04	105.80
33	BA	183	A	C8-N9-C4	5.59	108.04	105.80
33	BA	244	A	C4-C5-N7	-5.59	107.90	110.70
33	BA	637	A	C4-C5-N7	-5.59	107.90	110.70
33	BA	1119	A	C4-C5-N7	-5.59	107.90	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2071	A	C4-C5-N7	-5.59	107.90	110.70
33	BA	2317	A	C4-C5-N7	-5.59	107.90	110.70
33	BA	2461	A	C8-N9-C4	5.59	108.04	105.80
33	BA	2683	A	C4-C5-N7	-5.59	107.90	110.70
33	BA	2762	A	C8-N9-C4	5.59	108.04	105.80
1	AA	979	A	C8-N9-C4	5.59	108.04	105.80
1	AA	1115	A	C4-C5-N7	-5.59	107.90	110.70
33	BA	1149	A	C8-N9-C4	5.59	108.04	105.80
33	BA	1190	A	C8-N9-C4	5.59	108.04	105.80
33	BA	1381	A	C8-N9-C4	5.59	108.04	105.80
1	AA	799	A	C8-N9-C4	5.59	108.04	105.80
1	AA	879	A	C4-C5-C6	5.59	119.80	117.00
1	AA	917	A	C8-N9-C4	5.59	108.04	105.80
1	AA	1369	A	C8-N9-C4	5.59	108.04	105.80
1	AA	1509	A	C8-N9-C4	5.59	108.04	105.80
33	BA	193	A	C8-N9-C4	5.59	108.04	105.80
33	BA	740	A	N9-C4-C5	5.59	108.04	105.80
33	BA	1230	A	C8-N9-C4	5.59	108.04	105.80
33	BA	2152	A	N9-C4-C5	5.59	108.04	105.80
33	BA	2303	A	N9-C4-C5	5.59	108.04	105.80
33	BA	2462	A	C8-N9-C4	5.59	108.04	105.80
34	BB	56	A	C8-N9-C4	5.59	108.04	105.80
34	BB	114	A	C4-C5-N7	-5.59	107.90	110.70
1	AA	314	A	C8-N9-C4	5.59	108.03	105.80
1	AA	512	A	C8-N9-C4	5.59	108.04	105.80
1	AA	1160	A	C8-N9-C4	5.59	108.04	105.80
1	AA	1180	A	C8-N9-C4	5.59	108.03	105.80
33	BA	49	A	C4-C5-N7	-5.59	107.91	110.70
33	BA	108	A	C8-N9-C4	5.59	108.04	105.80
33	BA	1243	A	C4-C5-N7	-5.59	107.91	110.70
33	BA	1423	A	N9-C4-C5	5.59	108.04	105.80
33	BA	1456	A	N9-C4-C5	5.59	108.04	105.80
33	BA	1663	A	C8-N9-C4	5.59	108.04	105.80
33	BA	2479	A	C4-C5-C6	5.59	119.80	117.00
33	BA	67	A	N3-C4-N9	5.59	131.87	127.40
33	BA	1174	A	C4-C5-N7	-5.59	107.91	110.70
33	BA	1339	A	C4-C5-N7	-5.59	107.91	110.70
33	BA	1784	A	C4-C5-C6	5.59	119.79	117.00
33	BA	2216	A	C4-C5-N7	-5.59	107.91	110.70
33	BA	2375	A	N3-C4-N9	5.59	131.87	127.40
1	AA	160	A	C8-N9-C4	5.59	108.03	105.80
1	AA	508	A	C5-C6-N1	5.59	120.49	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	330	A	C8-N9-C4	5.59	108.03	105.80
33	BA	490	A	C4-C5-C6	5.59	119.79	117.00
33	BA	543	A	C8-N9-C4	5.59	108.03	105.80
33	BA	667	A	N3-C4-N9	5.59	131.87	127.40
33	BA	974	A	C8-N9-C4	5.59	108.03	105.80
33	BA	1123	A	C4-C5-C6	5.59	119.79	117.00
33	BA	1287	A	N9-C4-C5	5.59	108.03	105.80
33	BA	1592	A	C4-C5-N7	-5.59	107.91	110.70
33	BA	2526	A	C8-N9-C4	5.59	108.03	105.80
33	BA	2830	A	C8-N9-C4	5.59	108.03	105.80
1	AA	581	A	N9-C4-C5	5.58	108.03	105.80
1	AA	1349	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	1455	A	C8-N9-C4	5.58	108.03	105.80
33	BA	1055	A	C4-C5-N7	-5.58	107.91	110.70
33	BA	1957	A	N9-C4-C5	5.58	108.03	105.80
33	BA	2375	A	C4-C5-C6	5.58	119.79	117.00
1	AA	189	A	N3-C4-N9	5.58	131.87	127.40
1	AA	690	A	C8-N9-C4	5.58	108.03	105.80
1	AA	874	A	C8-N9-C4	5.58	108.03	105.80
1	AA	1014	A	C8-N9-C4	5.58	108.03	105.80
33	BA	224	A	C4-C5-N7	-5.58	107.91	110.70
33	BA	1302	A	C8-N9-C4	5.58	108.03	105.80
33	BA	2357	A	C4-C5-N7	-5.58	107.91	110.70
33	BA	2383	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	456	A	N9-C4-C5	5.58	108.03	105.80
33	BA	118	A	N3-C4-N9	5.58	131.87	127.40
33	BA	518	A	C8-N9-C4	5.58	108.03	105.80
33	BA	830	A	N9-C4-C5	5.58	108.03	105.80
33	BA	993	A	C8-N9-C4	5.58	108.03	105.80
33	BA	1653	A	C8-N9-C4	5.58	108.03	105.80
33	BA	2066	A	C8-N9-C4	5.58	108.03	105.80
33	BA	2307	A	N9-C4-C5	5.58	108.03	105.80
33	BA	2387	A	C8-N9-C4	5.58	108.03	105.80
33	BA	2661	A	C8-N9-C4	5.58	108.03	105.80
33	BA	2740	A	C8-N9-C4	5.58	108.03	105.80
33	BA	2887	A	C8-N9-C4	5.58	108.03	105.80
1	AA	978	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	1077	A	C4-C5-C6	5.58	119.79	117.00
1	AA	1486	A	C8-N9-C4	5.58	108.03	105.80
33	BA	652	A	N9-C4-C5	5.58	108.03	105.80
33	BA	922	A	N9-C4-C5	5.58	108.03	105.80
33	BA	1305	A	C4-C5-N7	-5.58	107.91	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2295	A	C4-C5-N7	-5.58	107.91	110.70
33	BA	2629	A	C8-N9-C4	5.58	108.03	105.80
1	AA	81	A	C8-N9-C4	5.58	108.03	105.80
1	AA	190	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	462	A	C8-N9-C4	5.58	108.03	105.80
1	AA	506	A	C8-N9-C4	5.58	108.03	105.80
1	AA	659	A	C8-N9-C4	5.58	108.03	105.80
1	AA	1120	A	C8-N9-C4	5.58	108.03	105.80
33	BA	41	A	C8-N9-C4	5.58	108.03	105.80
33	BA	44	A	C4-C5-N7	-5.58	107.91	110.70
33	BA	244	A	N9-C4-C5	5.58	108.03	105.80
33	BA	322	A	N9-C4-C5	5.58	108.03	105.80
33	BA	456	A	C8-N9-C4	5.58	108.03	105.80
33	BA	524	A	C8-N9-C4	5.58	108.03	105.80
33	BA	653	A	C8-N9-C4	5.58	108.03	105.80
33	BA	1021	A	C8-N9-C4	5.58	108.03	105.80
33	BA	1175	A	C4-C5-N7	-5.58	107.91	110.70
33	BA	1235	A	N9-C4-C5	5.58	108.03	105.80
33	BA	1302	A	C4-C5-C6	5.58	119.79	117.00
33	BA	1713	A	C4-C5-C6	5.58	119.79	117.00
33	BA	2480	A	N9-C4-C5	5.58	108.03	105.80
33	BA	2793	A	C8-N9-C4	5.58	108.03	105.80
33	BA	2837	A	C8-N9-C4	5.58	108.03	105.80
1	AA	323	A	C8-N9-C4	5.58	108.03	105.80
1	AA	582	A	N9-C4-C5	5.58	108.03	105.80
1	AA	1488	A	C8-N9-C4	5.58	108.03	105.80
33	BA	354	A	N3-C4-N9	5.58	131.86	127.40
33	BA	1175	A	N9-C4-C5	5.58	108.03	105.80
33	BA	1340	A	N9-C4-C5	5.58	108.03	105.80
33	BA	1499	A	N9-C4-C5	5.58	108.03	105.80
33	BA	1686	A	N9-C4-C5	5.58	108.03	105.80
1	AA	208	A	C8-N9-C4	5.58	108.03	105.80
1	AA	254	A	N9-C4-C5	5.58	108.03	105.80
1	AA	582	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	823	A	C8-N9-C4	5.58	108.03	105.80
1	AA	959	A	C8-N9-C4	5.58	108.03	105.80
1	AA	1403	A	C8-N9-C4	5.58	108.03	105.80
1	AA	1541	A	C4-C5-N7	-5.58	107.91	110.70
33	BA	1047	A	C4-C5-N7	-5.58	107.91	110.70
33	BA	1222	A	C8-N9-C4	5.58	108.03	105.80
33	BA	1593	A	C4-C5-N7	-5.58	107.91	110.70
33	BA	1695	A	C8-N9-C4	5.58	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1941	A	C4-C5-C6	5.58	119.79	117.00
33	BA	2663	A	C8-N9-C4	5.58	108.03	105.80
1	AA	178	A	N9-C4-C5	5.57	108.03	105.80
1	AA	433	A	C8-N9-C4	5.57	108.03	105.80
1	AA	704	A	C4-C5-N7	-5.57	107.91	110.70
33	BA	161	A	N3-C4-N9	5.57	131.86	127.40
33	BA	1054	A	C8-N9-C4	5.57	108.03	105.80
33	BA	1679	A	N9-C4-C5	5.57	108.03	105.80
33	BA	2262	A	C8-N9-C4	5.57	108.03	105.80
33	BA	2668	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	240	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	357	A	C4-C5-N7	-5.57	107.91	110.70
1	AA	703	A	C4-C5-N7	-5.57	107.91	110.70
33	BA	206	A	N9-C4-C5	5.57	108.03	105.80
33	BA	1115	A	C8-N9-C4	5.57	108.03	105.80
33	BA	2364	A	N9-C4-C5	5.57	108.03	105.80
1	AA	35	A	C8-N9-C4	5.57	108.03	105.80
1	AA	148	A	N9-C4-C5	5.57	108.03	105.80
1	AA	209	A	N9-C4-C5	5.57	108.03	105.80
33	BA	144	A	C8-N9-C4	5.57	108.03	105.80
33	BA	207	A	N3-C4-N9	5.57	131.86	127.40
33	BA	527	A	C4-C5-N7	-5.57	107.92	110.70
33	BA	925	A	C4-C5-N7	-5.57	107.91	110.70
33	BA	1685	A	C8-N9-C4	5.57	108.03	105.80
33	BA	1722	A	C8-N9-C4	5.57	108.03	105.80
33	BA	1844	A	C8-N9-C4	5.57	108.03	105.80
33	BA	1995	A	C8-N9-C4	5.57	108.03	105.80
33	BA	2191	A	N9-C4-C5	5.57	108.03	105.80
33	BA	2295	A	C8-N9-C4	5.57	108.03	105.80
1	AA	171	A	N9-C4-C5	5.57	108.03	105.80
1	AA	1289	A	C4-C5-C6	5.57	119.78	117.00
33	BA	110	A	C4-C5-N7	-5.57	107.92	110.70
33	BA	1314	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	438	A	C8-N9-C4	5.57	108.03	105.80
1	AA	669	A	C8-N9-C4	5.57	108.03	105.80
33	BA	199	A	C8-N9-C4	5.57	108.03	105.80
33	BA	1325	A	N9-C4-C5	5.57	108.03	105.80
33	BA	1654	A	N9-C4-C5	5.57	108.03	105.80
33	BA	2254	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	206	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	438	A	C4-C5-C6	5.57	119.78	117.00
1	AA	1206	A	C8-N9-C4	5.57	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1225	A	C4-C5-N7	-5.57	107.92	110.70
33	BA	154	A	C4-C5-N7	-5.57	107.92	110.70
33	BA	173	A	C8-N9-C4	5.57	108.03	105.80
33	BA	339	A	C8-N9-C4	5.57	108.03	105.80
33	BA	600	A	C8-N9-C4	5.57	108.03	105.80
33	BA	618	A	C8-N9-C4	5.57	108.03	105.80
33	BA	866	A	C8-N9-C4	5.57	108.03	105.80
33	BA	925	A	N9-C4-C5	5.57	108.03	105.80
33	BA	1029	A	C4-C5-N7	-5.57	107.92	110.70
33	BA	1254	A	C4-C5-N7	-5.57	107.92	110.70
33	BA	1483	A	N9-C4-C5	5.57	108.03	105.80
33	BA	1675	A	C8-N9-C4	5.57	108.03	105.80
33	BA	1844	A	C4-C5-N7	-5.57	107.92	110.70
33	BA	1876	A	N9-C4-C5	5.57	108.03	105.80
33	BA	2594	A	C4-C5-N7	-5.57	107.92	110.70
33	BA	470	A	N9-C4-C5	5.56	108.03	105.80
33	BA	723	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	1631	A	C8-N9-C4	5.56	108.03	105.80
33	BA	1679	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	2902	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	281	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	669	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	1443	A	C8-N9-C4	5.56	108.03	105.80
21	AX	23	A	C5-C6-N1	5.56	120.48	117.70
33	BA	12	A	C8-N9-C4	5.56	108.03	105.80
33	BA	273	A	N3-C4-N9	5.56	131.85	127.40
33	BA	273	A	C4-C5-C6	5.56	119.78	117.00
33	BA	274	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	322	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	723	A	C4-C5-C6	5.56	119.78	117.00
33	BA	1326	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	1361	A	C8-N9-C4	5.56	108.03	105.80
33	BA	1516	A	N9-C4-C5	5.56	108.03	105.80
33	BA	2071	A	N9-C4-C5	5.56	108.03	105.80
33	BA	2216	A	C8-N9-C4	5.56	108.03	105.80
1	AA	1294	A	C8-N9-C4	5.56	108.02	105.80
1	AA	1437	A	C8-N9-C4	5.56	108.02	105.80
33	BA	893	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	1812	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	31	A	N9-C4-C5	5.56	108.02	105.80
1	AA	924	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	21	A	C8-N9-C4	5.56	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	247	A	N9-C4-C5	5.56	108.02	105.80
33	BA	462	A	C8-N9-C4	5.56	108.02	105.80
33	BA	705	A	C8-N9-C4	5.56	108.02	105.80
33	BA	893	A	C8-N9-C4	5.56	108.02	105.80
33	BA	1115	A	N9-C4-C5	5.56	108.02	105.80
33	BA	1340	A	N3-C4-N9	5.56	131.85	127.40
33	BA	2078	A	C8-N9-C4	5.56	108.02	105.80
33	BA	2364	A	C8-N9-C4	5.56	108.02	105.80
33	BA	2618	A	C4-C5-C6	5.56	119.78	117.00
33	BA	2619	A	C8-N9-C4	5.56	108.02	105.80
33	BA	2750	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	541	A	C8-N9-C4	5.56	108.02	105.80
1	AA	1257	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	1419	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	326	A	C8-N9-C4	5.56	108.02	105.80
33	BA	345	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	727	A	C8-N9-C4	5.56	108.02	105.80
33	BA	753	A	C8-N9-C4	5.56	108.02	105.80
33	BA	1005	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	1055	A	N9-C4-C5	5.56	108.02	105.80
33	BA	1235	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	2134	A	C8-N9-C4	5.56	108.02	105.80
33	BA	2383	A	N9-C4-C5	5.56	108.02	105.80
1	AA	12	A	C8-N9-C4	5.56	108.02	105.80
1	AA	171	A	C8-N9-C4	5.56	108.02	105.80
1	AA	1272	A	C8-N9-C4	5.56	108.02	105.80
33	BA	500	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	1269	A	C4-C5-N7	-5.56	107.92	110.70
33	BA	1579	A	N3-C4-N9	5.56	131.84	127.40
33	BA	1784	A	C4-C5-N7	-5.56	107.92	110.70
1	AA	290	A	C8-N9-C4	5.55	108.02	105.80
1	AA	801	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	824	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	956	A	C8-N9-C4	5.55	108.02	105.80
1	AA	1502	A	N9-C4-C5	5.55	108.02	105.80
1	AA	1523	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	231	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	1243	A	N9-C4-C5	5.55	108.02	105.80
33	BA	1516	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	1929	A	C8-N9-C4	5.55	108.02	105.80
33	BA	1945	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	2835	A	C4-C5-N7	-5.55	107.92	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	959	A	N9-C4-C5	5.55	108.02	105.80
1	AA	1437	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	278	A	N9-C4-C5	5.55	108.02	105.80
33	BA	470	A	C8-N9-C4	5.55	108.02	105.80
33	BA	543	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	592	A	C8-N9-C4	5.55	108.02	105.80
33	BA	1699	A	C8-N9-C4	5.55	108.02	105.80
1	AA	72	A	C8-N9-C4	5.55	108.02	105.80
1	AA	452	A	C8-N9-C4	5.55	108.02	105.80
1	AA	556	A	C4-C5-C6	5.55	119.78	117.00
1	AA	690	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	929	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	1017	A	N9-C4-C5	5.55	108.02	105.80
33	BA	207	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	364	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	582	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	1277	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	1784	A	N3-C4-N9	5.55	131.84	127.40
33	BA	1831	A	C8-N9-C4	5.55	108.02	105.80
33	BA	2165	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	2329	A	C8-N9-C4	5.55	108.02	105.80
1	AA	61	A	C8-N9-C4	5.55	108.02	105.80
1	AA	690	A	N9-C4-C5	5.55	108.02	105.80
1	AA	1077	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	1103	A	C8-N9-C4	5.55	108.02	105.80
1	AA	1222	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	1238	A	C8-N9-C4	5.55	108.02	105.80
33	BA	428	A	C8-N9-C4	5.55	108.02	105.80
33	BA	1434	A	C4-C5-N7	-5.55	107.93	110.70
33	BA	1588	A	C8-N9-C4	5.55	108.02	105.80
33	BA	1982	A	C4-C5-N7	-5.55	107.92	110.70
33	BA	2018	A	C8-N9-C4	5.55	108.02	105.80
33	BA	2464	A	C8-N9-C4	5.55	108.02	105.80
1	AA	664	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	685	A	C8-N9-C4	5.55	108.02	105.80
1	AA	1050	A	C8-N9-C4	5.55	108.02	105.80
33	BA	325	A	C4-C5-N7	-5.55	107.93	110.70
33	BA	389	A	C4-C5-N7	-5.55	107.93	110.70
33	BA	2030	A	N9-C4-C5	5.55	108.02	105.80
33	BA	2187	A	N3-C4-N9	5.55	131.84	127.40
33	BA	2216	A	N9-C4-C5	5.55	108.02	105.80
33	BA	2869	A	N9-C4-C5	5.55	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	46	A	C8-N9-C4	5.55	108.02	105.80
1	AA	208	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	251	A	N9-C4-C5	5.55	108.02	105.80
1	AA	423	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	721	A	C8-N9-C4	5.55	108.02	105.80
1	AA	775	A	C8-N9-C4	5.55	108.02	105.80
1	AA	1422	A	N9-C4-C5	5.55	108.02	105.80
33	BA	5	A	C4-C5-N7	-5.55	107.93	110.70
33	BA	978	A	C4-C5-N7	-5.55	107.93	110.70
33	BA	1141	A	C4-C5-N7	-5.55	107.93	110.70
33	BA	1335	A	C8-N9-C4	5.55	108.02	105.80
1	AA	12	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	202	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	1502	A	C8-N9-C4	5.54	108.02	105.80
33	BA	407	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	1021	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	1534	A	C8-N9-C4	5.54	108.02	105.80
33	BA	2316	A	C8-N9-C4	5.54	108.02	105.80
33	BA	2673	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	148	A	C8-N9-C4	5.54	108.02	105.80
1	AA	287	A	C8-N9-C4	5.54	108.02	105.80
1	AA	381	A	C8-N9-C4	5.54	108.02	105.80
1	AA	925	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	1200	A	C8-N9-C4	5.54	108.02	105.80
33	BA	1189	A	N9-C4-C5	5.54	108.02	105.80
33	BA	2083	A	C4-C5-C6	5.54	119.77	117.00
33	BA	2191	A	C8-N9-C4	5.54	108.02	105.80
33	BA	2447	A	N9-C4-C5	5.54	108.02	105.80
33	BA	2463	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	240	A	N9-C4-C5	5.54	108.02	105.80
1	AA	501	A	N9-C4-C5	5.54	108.02	105.80
1	AA	803	A	N9-C4-C5	5.54	108.02	105.80
1	AA	902	A	C8-N9-C4	5.54	108.02	105.80
33	BA	207	A	N9-C4-C5	5.54	108.02	105.80
33	BA	1100	A	C8-N9-C4	5.54	108.02	105.80
33	BA	1631	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	2132	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	2270	A	C8-N9-C4	5.54	108.02	105.80
33	BA	2547	A	C8-N9-C4	5.54	108.02	105.80
33	BA	2834	A	N9-C4-C5	5.54	108.02	105.80
33	BA	2862	A	C8-N9-C4	5.54	108.02	105.80
33	BA	2900	A	C8-N9-C4	5.54	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	287	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	301	A	C8-N9-C4	5.54	108.02	105.80
1	AA	329	A	N9-C4-C5	5.54	108.02	105.80
1	AA	974	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	1333	A	N3-C4-N9	5.54	131.83	127.40
33	BA	126	A	N3-C4-N9	5.54	131.83	127.40
33	BA	314	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	1202	A	N9-C4-C5	5.54	108.02	105.80
33	BA	1456	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	28	A	C8-N9-C4	5.54	108.02	105.80
1	AA	53	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	401	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	415	A	N3-C4-N9	5.54	131.83	127.40
1	AA	638	A	C8-N9-C4	5.54	108.02	105.80
1	AA	1028	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	1386	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	1434	A	N9-C4-C5	5.54	108.02	105.80
33	BA	12	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	572	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	699	A	N9-C4-C5	5.54	108.02	105.80
33	BA	774	A	C4-C5-C6	5.54	119.77	117.00
33	BA	987	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	1464	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	2658	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	556	A	N3-C4-N9	5.54	131.83	127.40
1	AA	672	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	740	A	C8-N9-C4	5.54	108.02	105.80
33	BA	1084	A	N9-C4-C5	5.54	108.02	105.80
33	BA	1347	A	C8-N9-C4	5.54	108.02	105.80
33	BA	1553	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	1995	A	N9-C4-C5	5.54	108.02	105.80
33	BA	2464	A	N9-C4-C5	5.54	108.02	105.80
1	AA	150	A	C8-N9-C4	5.54	108.01	105.80
1	AA	500	A	C8-N9-C4	5.54	108.01	105.80
1	AA	1503	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	459	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	637	A	N9-C4-C5	5.54	108.01	105.80
33	BA	1617	A	C8-N9-C4	5.54	108.01	105.80
33	BA	1735	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	1812	A	C8-N9-C4	5.54	108.01	105.80
33	BA	1832	A	N9-C4-C5	5.54	108.01	105.80
33	BA	1982	A	N9-C4-C5	5.54	108.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2089	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	2105	U	N1-C2-O2	5.54	126.67	122.80
33	BA	2119	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	2700	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	2735	A	C8-N9-C4	5.54	108.01	105.80
33	BA	2835	A	N9-C4-C5	5.54	108.01	105.80
33	BA	2869	A	C4-C5-N7	-5.54	107.93	110.70
33	BA	2902	A	N9-C4-C5	5.54	108.01	105.80
1	AA	10	A	N9-C4-C5	5.53	108.01	105.80
1	AA	581	A	C4-C5-N7	-5.53	107.93	110.70
1	AA	630	A	N9-C4-C5	5.53	108.01	105.80
1	AA	649	A	C8-N9-C4	5.53	108.01	105.80
1	AA	771	A	C4-C5-N7	-5.53	107.93	110.70
1	AA	791	A	C8-N9-C4	5.53	108.01	105.80
1	AA	947	A	C4-C5-N7	-5.53	107.93	110.70
1	AA	1260	A	C8-N9-C4	5.53	108.01	105.80
1	AA	1417	A	C4-C5-N7	-5.53	107.93	110.70
33	BA	353	A	C4-C5-N7	-5.53	107.93	110.70
33	BA	469	A	C8-N9-C4	5.53	108.01	105.80
33	BA	470	A	C4-C5-N7	-5.53	107.93	110.70
33	BA	683	A	C4-C5-N7	-5.53	107.93	110.70
33	BA	1260	A	C4-C5-N7	-5.53	107.93	110.70
33	BA	2383	A	C8-N9-C4	5.53	108.01	105.80
33	BA	2601	A	N9-C4-C5	5.53	108.01	105.80
1	AA	1419	A	N9-C4-C5	5.53	108.01	105.80
33	BA	384	A	C4-C5-N7	-5.53	107.93	110.70
33	BA	978	A	N9-C4-C5	5.53	108.01	105.80
33	BA	2006	A	C8-N9-C4	5.53	108.01	105.80
1	AA	190	A	N9-C4-C5	5.53	108.01	105.80
1	AA	791	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	1140	A	N9-C4-C5	5.53	108.01	105.80
1	AA	1143	A	C8-N9-C4	5.53	108.01	105.80
33	BA	519	A	C4-C5-N7	-5.53	107.94	110.70
33	BA	702	A	C4-C5-N7	-5.53	107.93	110.70
33	BA	1141	A	N9-C4-C5	5.53	108.01	105.80
33	BA	1453	A	C8-N9-C4	5.53	108.01	105.80
1	AA	139	A	C8-N9-C4	5.53	108.01	105.80
1	AA	1523	A	N9-C4-C5	5.53	108.01	105.80
33	BA	584	A	C4-C5-N7	-5.53	107.94	110.70
33	BA	904	A	N9-C4-C5	5.53	108.01	105.80
33	BA	1541	A	C8-N9-C4	5.53	108.01	105.80
33	BA	1848	A	C8-N9-C4	5.53	108.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2762	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	721	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	1260	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	1523	A	C8-N9-C4	5.53	108.01	105.80
21	AX	14	A	C8-N9-C4	5.53	108.01	105.80
33	BA	279	A	C8-N9-C4	5.53	108.01	105.80
33	BA	889	A	C8-N9-C4	5.53	108.01	105.80
33	BA	1003	A	N9-C4-C5	5.53	108.01	105.80
33	BA	1059	A	C8-N9-C4	5.53	108.01	105.80
33	BA	1423	A	C8-N9-C4	5.53	108.01	105.80
33	BA	1499	A	C4-C5-N7	-5.53	107.94	110.70
33	BA	1534	A	C4-C5-N7	-5.53	107.94	110.70
33	BA	1580	A	C8-N9-C4	5.53	108.01	105.80
33	BA	1989	A	C8-N9-C4	5.53	108.01	105.80
33	BA	2089	A	N9-C4-C5	5.53	108.01	105.80
33	BA	2330	A	N3-C4-N9	5.53	131.82	127.40
33	BA	2777	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	28	A	N9-C4-C5	5.53	108.01	105.80
1	AA	55	A	C8-N9-C4	5.53	108.01	105.80
1	AA	251	A	C8-N9-C4	5.53	108.01	105.80
1	AA	415	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	918	A	C8-N9-C4	5.53	108.01	105.80
1	AA	1147	A	C4-C5-N7	-5.53	107.94	110.70
33	BA	124	A	C4-C5-N7	-5.53	107.94	110.70
33	BA	220	A	C4-C5-N7	-5.53	107.94	110.70
33	BA	575	A	C4-C5-C6	5.53	119.76	117.00
33	BA	647	A	N3-C4-N9	5.53	131.82	127.40
33	BA	1760	A	C8-N9-C4	5.53	108.01	105.80
33	BA	1956	A	N9-C4-C5	5.53	108.01	105.80
34	BB	76	A	C4-C5-N7	-5.53	107.94	110.70
34	BB	113	A	C8-N9-C4	5.53	108.01	105.80
1	AA	738	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	1115	A	N9-C4-C5	5.52	108.01	105.80
33	BA	166	A	N9-C4-C5	5.52	108.01	105.80
33	BA	908	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2908	A	N9-C4-C5	5.52	108.01	105.80
1	AA	203	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	500	A	N3-C4-N9	5.52	131.82	127.40
1	AA	669	A	N9-C4-C5	5.52	108.01	105.80
1	AA	816	A	N9-C4-C5	5.52	108.01	105.80
1	AA	1121	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	1437	A	N9-C4-C5	5.52	108.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	124	A	N9-C4-C5	5.52	108.01	105.80
33	BA	342	A	N9-C4-C5	5.52	108.01	105.80
33	BA	722	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	847	A	C4-C5-C6	5.52	119.76	117.00
33	BA	1346	A	N9-C4-C5	5.52	108.01	105.80
33	BA	1465	A	C8-N9-C4	5.52	108.01	105.80
33	BA	1818	A	C8-N9-C4	5.52	108.01	105.80
33	BA	2170	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2307	A	C8-N9-C4	5.52	108.01	105.80
33	BA	2338	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2351	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2740	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	684	A	C8-N9-C4	5.52	108.01	105.80
1	AA	923	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	1185	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	1510	A	C8-N9-C4	5.52	108.01	105.80
33	BA	746	A	C8-N9-C4	5.52	108.01	105.80
33	BA	965	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2769	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2904	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	337	A	C8-N9-C4	5.52	108.01	105.80
1	AA	651	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	791	A	N9-C4-C5	5.52	108.01	105.80
1	AA	1403	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	73	A	N9-C4-C5	5.52	108.01	105.80
33	BA	429	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	867	A	N9-C4-C5	5.52	108.01	105.80
33	BA	1061	A	N3-C4-N9	5.52	131.82	127.40
33	BA	1210	A	C8-N9-C4	5.52	108.01	105.80
33	BA	2018	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2091	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2100	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2643	A	C8-N9-C4	5.52	108.01	105.80
33	BA	2670	A	C4-C5-C6	5.52	119.76	117.00
33	BA	2845	A	N9-C4-C5	5.52	108.01	105.80
1	AA	474	A	C8-N9-C4	5.52	108.01	105.80
1	AA	1054	A	C8-N9-C4	5.52	108.01	105.80
1	AA	1359	A	C4-C5-N7	-5.52	107.94	110.70
21	AX	44	A	C8-N9-C4	5.52	108.01	105.80
33	BA	179	A	N3-C4-N9	5.52	131.81	127.40
33	BA	274	A	N9-C4-C5	5.52	108.01	105.80
33	BA	428	A	C4-C5-N7	-5.52	107.94	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1144	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	1224	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	1230	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	1286	A	C8-N9-C4	5.52	108.01	105.80
33	BA	1601	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	1617	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	1709	A	C8-N9-C4	5.52	108.01	105.80
33	BA	1995	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2298	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2395	A	C8-N9-C4	5.52	108.01	105.80
1	AA	107	A	C4-C5-N7	-5.52	107.94	110.70
1	AA	140	A	C8-N9-C4	5.52	108.01	105.80
1	AA	271	A	N9-C4-C5	5.52	108.01	105.80
33	BA	268	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	342	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	1092	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	1838	A	N9-C4-C5	5.52	108.01	105.80
33	BA	2220	A	C8-N9-C4	5.52	108.01	105.80
33	BA	2375	A	C4-C5-N7	-5.52	107.94	110.70
33	BA	2837	A	N9-C4-C5	5.52	108.01	105.80
1	AA	282	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	475	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	968	A	N9-C4-C5	5.51	108.01	105.80
1	AA	1529	A	C4-C5-N7	-5.51	107.94	110.70
33	BA	229	A	C4-C5-N7	-5.51	107.94	110.70
33	BA	479	A	C4-C5-N7	-5.51	107.94	110.70
33	BA	678	A	N9-C4-C5	5.51	108.01	105.80
33	BA	758	A	C4-C5-N7	-5.51	107.94	110.70
33	BA	1620	A	C8-N9-C4	5.51	108.01	105.80
33	BA	1724	A	N9-C4-C5	5.51	108.01	105.80
33	BA	1797	A	C8-N9-C4	5.51	108.01	105.80
33	BA	2362	A	N9-C4-C5	5.51	108.01	105.80
34	BB	43	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	204	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	738	A	N9-C4-C5	5.51	108.00	105.80
21	AX	44	A	C4-C5-N7	-5.51	107.94	110.70
33	BA	2804	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	160	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	544	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	705	A	C8-N9-C4	5.51	108.00	105.80
1	AA	928	A	N9-C4-C5	5.51	108.00	105.80
33	BA	14	A	N9-C4-C5	5.51	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	518	A	C4-C5-N7	-5.51	107.94	110.70
33	BA	811	A	C8-N9-C4	5.51	108.00	105.80
33	BA	1142	A	C4-C5-N7	-5.51	107.94	110.70
33	BA	1221	A	C8-N9-C4	5.51	108.00	105.80
33	BA	1942	A	C4-C5-N7	-5.51	107.94	110.70
33	BA	2327	A	C8-N9-C4	5.51	108.00	105.80
1	AA	225	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	329	A	C8-N9-C4	5.51	108.00	105.80
1	AA	713	A	C8-N9-C4	5.51	108.00	105.80
1	AA	1266	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	1320	A	C8-N9-C4	5.51	108.00	105.80
1	AA	1417	A	N9-C4-C5	5.51	108.00	105.80
1	AA	1425	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	1466	A	C4-C5-N7	-5.51	107.94	110.70
33	BA	275	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	543	A	N9-C4-C5	5.51	108.00	105.80
33	BA	560	A	N9-C4-C5	5.51	108.00	105.80
33	BA	987	A	N9-C4-C5	5.51	108.00	105.80
33	BA	1809	A	N9-C4-C5	5.51	108.00	105.80
33	BA	2402	A	C8-N9-C4	5.51	108.00	105.80
33	BA	2606	A	C8-N9-C4	5.51	108.00	105.80
33	BA	2683	A	N9-C4-C5	5.51	108.00	105.80
33	BA	2782	A	C8-N9-C4	5.51	108.00	105.80
33	BA	2907	A	N9-C4-C5	5.51	108.00	105.80
34	BB	37	A	N9-C4-C5	5.51	108.00	105.80
34	BB	56	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	1259	A	C4-C5-N7	-5.51	107.95	110.70
1	AA	1422	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	178	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	1132	A	N9-C4-C5	5.51	108.00	105.80
33	BA	2570	A	C4-C5-N7	-5.51	107.95	110.70
1	AA	232	A	N3-C4-N9	5.51	131.81	127.40
1	AA	507	A	C4-C5-C6	5.51	119.75	117.00
1	AA	777	A	C4-C5-N7	-5.51	107.95	110.70
1	AA	801	A	N9-C4-C5	5.51	108.00	105.80
1	AA	1103	A	C4-C5-N7	-5.51	107.95	110.70
1	AA	1147	A	N9-C4-C5	5.51	108.00	105.80
1	AA	1478	A	C8-N9-C4	5.51	108.00	105.80
1	AA	1513	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	449	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	477	A	N3-C4-N9	5.51	131.81	127.40
33	BA	723	A	N3-C4-N9	5.51	131.81	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1055	A	C8-N9-C4	5.51	108.00	105.80
33	BA	1313	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	1346	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	1445	A	C8-N9-C4	5.51	108.00	105.80
33	BA	1583	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	1697	A	C8-N9-C4	5.51	108.00	105.80
33	BA	1832	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	1918	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	2405	A	C4-C5-N7	-5.51	107.95	110.70
33	BA	2479	A	N9-C4-C5	5.51	108.00	105.80
1	AA	99	A	C8-N9-C4	5.50	108.00	105.80
1	AA	367	A	C8-N9-C4	5.50	108.00	105.80
21	AX	41	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	2083	A	C5-C6-N1	5.50	120.45	117.70
33	BA	2176	A	C4-C5-N7	-5.50	107.95	110.70
34	BB	27	A	N9-C4-C5	5.50	108.00	105.80
1	AA	592	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	924	A	C8-N9-C4	5.50	108.00	105.80
1	AA	1111	A	N9-C4-C5	5.50	108.00	105.80
1	AA	1456	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	140	A	N9-C4-C5	5.50	108.00	105.80
33	BA	222	A	C8-N9-C4	5.50	108.00	105.80
33	BA	259	A	C8-N9-C4	5.50	108.00	105.80
33	BA	281	A	C8-N9-C4	5.50	108.00	105.80
33	BA	431	A	C8-N9-C4	5.50	108.00	105.80
33	BA	449	A	C8-N9-C4	5.50	108.00	105.80
33	BA	769	A	C8-N9-C4	5.50	108.00	105.80
33	BA	821	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	876	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	1201	A	C8-N9-C4	5.50	108.00	105.80
33	BA	1788	A	N9-C4-C5	5.50	108.00	105.80
33	BA	1981	A	N9-C4-C5	5.50	108.00	105.80
33	BA	2146	A	N9-C4-C5	5.50	108.00	105.80
1	AA	228	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	254	A	N3-C4-N9	5.50	131.80	127.40
1	AA	786	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	1207	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	1510	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	10	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	893	A	N9-C4-C5	5.50	108.00	105.80
33	BA	1067	A	C4-C5-C6	5.50	119.75	117.00
33	BA	1103	A	C8-N9-C4	5.50	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1426	A	C8-N9-C4	5.50	108.00	105.80
33	BA	1580	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	1686	A	C8-N9-C4	5.50	108.00	105.80
33	BA	2570	A	C8-N9-C4	5.50	108.00	105.80
33	BA	2904	A	C8-N9-C4	5.50	108.00	105.80
1	AA	225	A	N9-C4-C5	5.50	108.00	105.80
1	AA	913	A	C8-N9-C4	5.50	108.00	105.80
1	AA	1161	A	C8-N9-C4	5.50	108.00	105.80
1	AA	1422	A	N3-C4-N9	5.50	131.80	127.40
21	AX	21	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	61	A	C8-N9-C4	5.50	108.00	105.80
33	BA	150	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	173	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	1244	A	N9-C4-C5	5.50	108.00	105.80
33	BA	2601	A	N3-C4-N9	5.50	131.80	127.40
33	BA	2629	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	210	A	C8-N9-C4	5.50	108.00	105.80
1	AA	333	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	419	A	N3-C4-N9	5.50	131.80	127.40
1	AA	518	A	N9-C4-C5	5.50	108.00	105.80
1	AA	1425	A	C8-N9-C4	5.50	108.00	105.80
33	BA	231	A	N9-C4-C5	5.50	108.00	105.80
33	BA	412	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	677	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	1592	A	N9-C4-C5	5.50	108.00	105.80
33	BA	1677	A	C8-N9-C4	5.50	108.00	105.80
33	BA	1956	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	1965	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	1966	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	2100	A	N9-C4-C5	5.50	108.00	105.80
33	BA	2767	A	N9-C4-C5	5.50	108.00	105.80
33	BA	2779	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	2819	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	2854	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	2875	A	C8-N9-C4	5.50	108.00	105.80
34	BB	18	A	C8-N9-C4	5.50	108.00	105.80
1	AA	171	A	C4-C5-N7	-5.50	107.95	110.70
1	AA	541	A	N9-C4-C5	5.50	108.00	105.80
1	AA	583	A	N3-C4-N9	5.50	131.80	127.40
1	AA	945	A	C8-N9-C4	5.50	108.00	105.80
1	AA	985	A	C4-C5-C6	5.50	119.75	117.00
33	BA	436	A	C4-C5-N7	-5.50	107.95	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1026	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	1734	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	1745	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	1791	A	N9-C4-C5	5.50	108.00	105.80
33	BA	1888	A	C8-N9-C4	5.50	108.00	105.80
33	BA	2924	A	C8-N9-C4	5.50	108.00	105.80
34	BB	50	A	C8-N9-C4	5.50	108.00	105.80
1	AA	372	A	C8-N9-C4	5.50	108.00	105.80
1	AA	401	A	N9-C4-C5	5.50	108.00	105.80
1	AA	757	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	52	A	C4-C5-N7	-5.50	107.95	110.70
33	BA	965	A	N9-C4-C5	5.50	108.00	105.80
33	BA	1579	A	C4-C5-C6	5.50	119.75	117.00
33	BA	2062	A	C4-C5-C6	5.50	119.75	117.00
1	AA	440	A	N9-C4-C5	5.49	108.00	105.80
1	AA	1090	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	1112	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	1297	A	C8-N9-C4	5.49	108.00	105.80
33	BA	198	A	C8-N9-C4	5.49	108.00	105.80
33	BA	219	A	C4-C5-N7	-5.49	107.95	110.70
33	BA	220	A	N9-C4-C5	5.49	108.00	105.80
33	BA	572	A	N9-C4-C5	5.49	108.00	105.80
33	BA	922	A	C8-N9-C4	5.49	108.00	105.80
33	BA	1066	A	C4-C5-N7	-5.49	107.95	110.70
33	BA	1697	A	C4-C5-N7	-5.49	107.95	110.70
33	BA	2387	A	C4-C5-N7	-5.49	107.95	110.70
33	BA	2571	A	N9-C4-C5	5.49	108.00	105.80
33	BA	345	A	N9-C4-C5	5.49	108.00	105.80
33	BA	384	A	N9-C4-C5	5.49	108.00	105.80
33	BA	2018	A	N9-C4-C5	5.49	108.00	105.80
1	AA	225	A	C8-N9-C4	5.49	108.00	105.80
1	AA	1028	A	N9-C4-C5	5.49	108.00	105.80
1	AA	1257	A	N9-C4-C5	5.49	108.00	105.80
1	AA	1509	A	C4-C5-N7	-5.49	107.95	110.70
33	BA	102	A	C4-C5-N7	-5.49	107.95	110.70
33	BA	254	A	C5-C6-N1	5.49	120.45	117.70
33	BA	479	A	N9-C4-C5	5.49	108.00	105.80
33	BA	575	A	N3-C4-N9	5.49	131.79	127.40
33	BA	646	A	C4-C5-N7	-5.49	107.95	110.70
33	BA	829	A	C4-C5-N7	-5.49	107.95	110.70
33	BA	2089	A	C4-C5-C6	5.49	119.75	117.00
33	BA	2220	A	N9-C4-C5	5.49	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2462	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	321	A	C8-N9-C4	5.49	108.00	105.80
1	AA	323	A	N9-C4-C5	5.49	108.00	105.80
1	AA	828	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	1006	A	N9-C4-C5	5.49	108.00	105.80
33	BA	65	A	C8-N9-C4	5.49	108.00	105.80
33	BA	418	A	N9-C4-C5	5.49	108.00	105.80
33	BA	548	A	C4-C5-N7	-5.49	107.95	110.70
33	BA	987	A	C8-N9-C4	5.49	108.00	105.80
33	BA	1230	A	N9-C4-C5	5.49	108.00	105.80
33	BA	2898	A	C8-N9-C4	5.49	108.00	105.80
33	BA	2908	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	52	A	C8-N9-C4	5.49	108.00	105.80
33	BA	176	A	C8-N9-C4	5.49	108.00	105.80
33	BA	2317	A	N9-C4-C5	5.49	108.00	105.80
1	AA	569	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	592	A	N9-C4-C5	5.49	107.99	105.80
1	AA	775	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	1205	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	1247	A	C8-N9-C4	5.49	108.00	105.80
1	AA	1248	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	1372	A	C8-N9-C4	5.49	107.99	105.80
33	BA	1027	A	C8-N9-C4	5.49	107.99	105.80
33	BA	1631	A	N9-C4-C5	5.49	108.00	105.80
33	BA	2088	A	C4-C5-N7	-5.49	107.96	110.70
33	BA	2406	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	142	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	287	A	N9-C4-C5	5.48	107.99	105.80
1	AA	1254	A	N9-C4-C5	5.48	107.99	105.80
33	BA	354	A	N9-C4-C5	5.48	107.99	105.80
33	BA	2923	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	793	A	C8-N9-C4	5.48	107.99	105.80
1	AA	925	A	N9-C4-C5	5.48	107.99	105.80
1	AA	1180	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	1384	A	C8-N9-C4	5.48	107.99	105.80
33	BA	154	A	N9-C4-C5	5.48	107.99	105.80
33	BA	202	A	N9-C4-C5	5.48	107.99	105.80
33	BA	622	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	763	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	1179	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	1190	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	1585	A	C4-C5-N7	-5.48	107.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1745	A	N9-C4-C5	5.48	107.99	105.80
33	BA	1788	A	C8-N9-C4	5.48	107.99	105.80
33	BA	2030	A	C8-N9-C4	5.48	107.99	105.80
33	BA	2256	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	2904	A	N9-C4-C5	5.48	107.99	105.80
34	BB	105	A	C8-N9-C4	5.48	107.99	105.80
1	AA	254	A	C4-C5-C6	5.48	119.74	117.00
1	AA	357	A	N9-C4-C5	5.48	107.99	105.80
1	AA	638	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	537	A	C8-N9-C4	5.48	107.99	105.80
33	BA	957	A	C8-N9-C4	5.48	107.99	105.80
33	BA	999	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	1339	A	N9-C4-C5	5.48	107.99	105.80
33	BA	2155	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	457	A	N3-C4-N9	5.48	131.78	127.40
1	AA	658	A	N9-C4-C5	5.48	107.99	105.80
1	AA	825	A	N9-C4-C5	5.48	107.99	105.80
33	BA	1078	A	C8-N9-C4	5.48	107.99	105.80
33	BA	1312	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	1627	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	1815	A	N9-C4-C5	5.48	107.99	105.80
33	BA	1885	A	C8-N9-C4	5.48	107.99	105.80
33	BA	2356	A	N9-C4-C5	5.48	107.99	105.80
33	BA	2898	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	886	A	N9-C4-C5	5.48	107.99	105.80
1	AA	1442	A	C4-C5-N7	-5.48	107.96	110.70
21	AX	58	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	12	A	N9-C4-C5	5.48	107.99	105.80
33	BA	14	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	91	A	N9-C4-C5	5.48	107.99	105.80
33	BA	210	A	N9-C4-C5	5.48	107.99	105.80
33	BA	231	A	C8-N9-C4	5.48	107.99	105.80
33	BA	275	A	N9-C4-C5	5.48	107.99	105.80
33	BA	353	A	N9-C4-C5	5.48	107.99	105.80
33	BA	376	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	593	A	N9-C4-C5	5.48	107.99	105.80
33	BA	600	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	917	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	1074	A	C8-N9-C4	5.48	107.99	105.80
33	BA	1677	A	N9-C4-C5	5.48	107.99	105.80
33	BA	1802	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	1981	A	C4-C5-N7	-5.48	107.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2049	A	C8-N9-C4	5.48	107.99	105.80
33	BA	2834	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	171	A	C4-C5-C6	5.48	119.74	117.00
1	AA	1528	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	314	A	N9-C4-C5	5.48	107.99	105.80
33	BA	971	A	C8-N9-C4	5.48	107.99	105.80
33	BA	1021	A	N9-C4-C5	5.48	107.99	105.80
33	BA	1059	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	1858	A	C8-N9-C4	5.48	107.99	105.80
33	BA	1957	A	C8-N9-C4	5.48	107.99	105.80
33	BA	2767	A	C4-C5-N7	-5.48	107.96	110.70
33	BA	2845	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	743	A	C8-N9-C4	5.47	107.99	105.80
1	AA	1147	A	C8-N9-C4	5.47	107.99	105.80
1	AA	1213	A	C8-N9-C4	5.47	107.99	105.80
1	AA	1493	A	C4-C5-N7	-5.47	107.96	110.70
33	BA	118	A	N9-C4-C5	5.47	107.99	105.80
33	BA	549	A	C4-C5-N7	-5.47	107.96	110.70
33	BA	732	A	C4-C5-C6	5.47	119.74	117.00
33	BA	1405	A	C4-C5-N7	-5.47	107.96	110.70
33	BA	1542	A	N9-C4-C5	5.47	107.99	105.80
33	BA	1588	A	C4-C5-N7	-5.47	107.96	110.70
33	BA	1905	A	N3-C4-N9	5.47	131.78	127.40
33	BA	2146	A	C4-C5-N7	-5.47	107.96	110.70
33	BA	2629	A	N9-C4-C5	5.47	107.99	105.80
1	AA	62	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	475	A	N9-C4-C5	5.47	107.99	105.80
1	AA	541	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	762	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	775	A	C4-C5-C6	5.47	119.74	117.00
1	AA	777	A	N9-C4-C5	5.47	107.99	105.80
1	AA	1271	A	C4-C5-N7	-5.47	107.96	110.70
33	BA	364	A	N9-C4-C5	5.47	107.99	105.80
33	BA	1034	A	C4-C5-N7	-5.47	107.96	110.70
33	BA	1636	A	C4-C5-N7	-5.47	107.96	110.70
33	BA	1636	A	N9-C4-C5	5.47	107.99	105.80
33	BA	1723	A	C8-N9-C4	5.47	107.99	105.80
33	BA	2436	A	C8-N9-C4	5.47	107.99	105.80
1	AA	460	A	C4-C5-N7	-5.47	107.97	110.70
21	AX	14	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	279	A	N9-C4-C5	5.47	107.99	105.80
33	BA	1243	A	C8-N9-C4	5.47	107.99	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1957	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	2356	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	2571	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	618	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	996	A	C8-N9-C4	5.47	107.99	105.80
1	AA	1004	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	173	A	N9-C4-C5	5.47	107.99	105.80
33	BA	307	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	373	A	C8-N9-C4	5.47	107.99	105.80
33	BA	1266	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	1393	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	1540	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	1914	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	1966	A	N9-C4-C5	5.47	107.99	105.80
33	BA	2089	A	N3-C4-N9	5.47	131.78	127.40
33	BA	2176	A	N9-C4-C5	5.47	107.99	105.80
33	BA	2441	A	C8-N9-C4	5.47	107.99	105.80
33	BA	2511	A	C4-C5-N7	-5.47	107.97	110.70
34	BB	71	A	N9-C4-C5	5.47	107.99	105.80
1	AA	776	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	653	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	851	A	N9-C4-C5	5.47	107.99	105.80
33	BA	958	A	N9-C4-C5	5.47	107.99	105.80
33	BA	1593	A	N9-C4-C5	5.47	107.99	105.80
33	BA	2262	A	N3-C4-N9	5.47	131.78	127.40
33	BA	2507	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	209	A	N3-C4-N9	5.47	131.77	127.40
1	AA	1283	A	C4-C5-N7	-5.47	107.97	110.70
33	BA	162	A	C8-N9-C4	5.47	107.99	105.80
33	BA	389	A	N9-C4-C5	5.47	107.99	105.80
33	BA	479	A	C8-N9-C4	5.47	107.99	105.80
33	BA	811	A	N3-C4-N9	5.47	131.77	127.40
33	BA	847	A	N3-C4-N9	5.47	131.77	127.40
33	BA	1534	A	N9-C4-C5	5.47	107.99	105.80
33	BA	2220	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	210	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	210	A	N9-C4-C5	5.46	107.99	105.80
1	AA	386	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	522	A	N9-C4-C5	5.46	107.99	105.80
1	AA	917	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1283	A	N9-C4-C5	5.46	107.99	105.80
33	BA	407	A	N9-C4-C5	5.46	107.99	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	500	A	N9-C4-C5	5.46	107.99	105.80
33	BA	835	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	1130	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	1838	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	2030	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	2060	A	N9-C4-C5	5.46	107.99	105.80
33	BA	2205	A	C8-N9-C4	5.46	107.99	105.80
33	BA	551	A	C8-N9-C4	5.46	107.98	105.80
33	BA	1078	A	N3-C4-N9	5.46	131.77	127.40
33	BA	1930	A	C8-N9-C4	5.46	107.98	105.80
1	AA	12	A	N9-C4-C5	5.46	107.98	105.80
1	AA	542	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1178	A	C8-N9-C4	5.46	107.98	105.80
1	AA	1266	A	N9-C4-C5	5.46	107.98	105.80
33	BA	176	A	N9-C4-C5	5.46	107.98	105.80
33	BA	302	A	C8-N9-C4	5.46	107.98	105.80
33	BA	952	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	1746	A	N9-C4-C5	5.46	107.98	105.80
33	BA	1906	A	N9-C4-C5	5.46	107.98	105.80
33	BA	2027	A	C8-N9-C4	5.46	107.98	105.80
33	BA	2762	A	N9-C4-C5	5.46	107.98	105.80
1	AA	271	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	968	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1056	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1179	A	C8-N9-C4	5.46	107.98	105.80
1	AA	1425	A	N9-C4-C5	5.46	107.98	105.80
33	BA	1277	A	N9-C4-C5	5.46	107.98	105.80
33	BA	1677	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	2390	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	202	A	N9-C4-C5	5.46	107.98	105.80
1	AA	532	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1120	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1140	A	C8-N9-C4	5.46	107.98	105.80
33	BA	71	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	144	A	N9-C4-C5	5.46	107.98	105.80
33	BA	337	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	616	A	C8-N9-C4	5.46	107.98	105.80
33	BA	770	A	N9-C4-C5	5.46	107.98	105.80
33	BA	840	A	C6-N1-C2	-5.46	115.33	118.60
33	BA	1130	A	C8-N9-C4	5.46	107.98	105.80
33	BA	1142	A	N9-C4-C5	5.46	107.98	105.80
33	BA	1265	A	N9-C4-C5	5.46	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1323	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	1636	A	C8-N9-C4	5.46	107.98	105.80
33	BA	2227	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	2686	A	N9-C4-C5	5.46	107.98	105.80
1	AA	258	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1435	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	130	A	C8-N9-C4	5.46	107.98	105.80
33	BA	373	A	N9-C4-C5	5.46	107.98	105.80
33	BA	507	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	548	A	N9-C4-C5	5.46	107.98	105.80
33	BA	623	A	C8-N9-C4	5.46	107.98	105.80
33	BA	1144	A	N9-C4-C5	5.46	107.98	105.80
33	BA	1930	A	N9-C4-C5	5.46	107.98	105.80
33	BA	1961	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	2141	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	2170	A	N9-C4-C5	5.46	107.98	105.80
33	BA	2254	A	N3-C4-N9	5.46	131.76	127.40
33	BA	2827	A	C8-N9-C4	5.46	107.98	105.80
33	BA	2846	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	390	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	518	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	713	A	N9-C4-C5	5.46	107.98	105.80
33	BA	206	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	207	A	C4-C5-C6	5.46	119.73	117.00
33	BA	548	A	C8-N9-C4	5.46	107.98	105.80
33	BA	1003	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	1434	A	N3-C4-N9	5.46	131.76	127.40
33	BA	1465	A	N9-C4-C5	5.46	107.98	105.80
33	BA	1789	A	N9-C4-C5	5.46	107.98	105.80
33	BA	1813	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	1885	A	C4-C5-N7	-5.46	107.97	110.70
33	BA	2297	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	151	A	C8-N9-C4	5.45	107.98	105.80
1	AA	159	A	N9-C4-C5	5.45	107.98	105.80
1	AA	306	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	306	A	N9-C4-C5	5.45	107.98	105.80
1	AA	397	A	C8-N9-C4	5.45	107.98	105.80
1	AA	837	A	N9-C4-C5	5.45	107.98	105.80
1	AA	1503	A	N9-C4-C5	5.45	107.98	105.80
33	BA	469	A	C4-C5-N7	-5.45	107.97	110.70
33	BA	658	A	C4-C5-N7	-5.45	107.97	110.70
33	BA	808	A	C4-C5-N7	-5.45	107.97	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1818	A	N9-C4-C5	5.45	107.98	105.80
33	BA	2590	A	C8-N9-C4	5.45	107.98	105.80
34	BB	37	A	C8-N9-C4	5.45	107.98	105.80
34	BB	55	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	195	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	1210	A	C4-C5-N7	-5.45	107.97	110.70
33	BA	222	A	N9-C4-C5	5.45	107.98	105.80
33	BA	355	A	N9-C4-C5	5.45	107.98	105.80
33	BA	1123	A	C4-C5-N7	-5.45	107.97	110.70
33	BA	1347	A	N3-C4-N9	5.45	131.76	127.40
33	BA	2570	A	N9-C4-C5	5.45	107.98	105.80
1	AA	236	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	439	A	C5-C6-N1	5.45	120.42	117.70
1	AA	644	A	C8-N9-C4	5.45	107.98	105.80
1	AA	721	A	N9-C4-C5	5.45	107.98	105.80
1	AA	758	A	C8-N9-C4	5.45	107.98	105.80
1	AA	825	A	C8-N9-C4	5.45	107.98	105.80
1	AA	1358	A	C5-C6-N1	5.45	120.42	117.70
1	AA	1541	A	N9-C4-C5	5.45	107.98	105.80
21	AX	76	A	C8-N9-C4	5.45	107.98	105.80
33	BA	56	A	C5-C6-N1	5.45	120.42	117.70
33	BA	73	A	C4-C5-N7	-5.45	107.97	110.70
33	BA	193	A	C4-C5-N7	-5.45	107.97	110.70
33	BA	574	A	N9-C4-C5	5.45	107.98	105.80
33	BA	661	A	C8-N9-C4	5.45	107.98	105.80
33	BA	690	A	C4-C5-N7	-5.45	107.97	110.70
33	BA	1724	A	C8-N9-C4	5.45	107.98	105.80
33	BA	2052	A	C4-C5-N7	-5.45	107.97	110.70
33	BA	2593	A	C4-C5-N7	-5.45	107.97	110.70
33	BA	2618	A	N3-C4-N9	5.45	131.76	127.40
33	BA	2700	A	N9-C4-C5	5.45	107.98	105.80
34	BB	39	A	N9-C4-C5	5.45	107.98	105.80
1	AA	281	A	N9-C4-C5	5.45	107.98	105.80
1	AA	1004	A	C8-N9-C4	5.45	107.98	105.80
1	AA	1207	A	N9-C4-C5	5.45	107.98	105.80
21	AX	23	A	N9-C4-C5	5.45	107.98	105.80
33	BA	130	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	438	A	N9-C4-C5	5.45	107.98	105.80
33	BA	947	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	1019	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	1697	A	N9-C4-C5	5.45	107.98	105.80
33	BA	1699	A	C4-C5-N7	-5.45	107.98	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1906	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	2034	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	2389	A	C8-N9-C4	5.45	107.98	105.80
33	BA	2477	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	2673	A	N9-C4-C5	5.45	107.98	105.80
1	AA	715	A	C4-C5-N7	-5.45	107.98	110.70
1	AA	919	A	N9-C4-C5	5.45	107.98	105.80
1	AA	1289	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	95	A	C8-N9-C4	5.45	107.98	105.80
33	BA	974	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	1504	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	1746	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	1989	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	2006	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	2315	A	N9-C4-C5	5.45	107.98	105.80
1	AA	1017	A	C4-C5-N7	-5.45	107.98	110.70
1	AA	1133	A	C4-C5-C6	5.45	119.72	117.00
33	BA	782	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	1066	A	N9-C4-C5	5.45	107.98	105.80
33	BA	1314	A	N9-C4-C5	5.45	107.98	105.80
33	BA	1346	A	C8-N9-C4	5.45	107.98	105.80
33	BA	1381	A	N9-C4-C5	5.45	107.98	105.80
33	BA	1499	A	C8-N9-C4	5.45	107.98	105.80
33	BA	1524	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	2276	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	2327	A	C4-C5-N7	-5.45	107.98	110.70
33	BA	2643	A	N9-C4-C5	5.45	107.98	105.80
1	AA	569	A	N9-C4-C5	5.44	107.98	105.80
1	AA	1090	A	N9-C4-C5	5.44	107.98	105.80
1	AA	1386	A	N9-C4-C5	5.44	107.98	105.80
33	BA	10	A	N9-C4-C5	5.44	107.98	105.80
33	BA	222	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	1014	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	1036	A	C8-N9-C4	5.44	107.98	105.80
33	BA	1542	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	1913	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	1948	A	N9-C4-C5	5.44	107.98	105.80
33	BA	2479	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	2480	A	C8-N9-C4	5.44	107.98	105.80
1	AA	270	A	C8-N9-C4	5.44	107.98	105.80
1	AA	296	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	715	A	N9-C4-C5	5.44	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1140	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	1510	A	N9-C4-C5	5.44	107.98	105.80
33	BA	49	A	C8-N9-C4	5.44	107.98	105.80
33	BA	333	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	699	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	999	A	N9-C4-C5	5.44	107.98	105.80
33	BA	1260	A	N9-C4-C5	5.44	107.98	105.80
33	BA	1533	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	2006	A	N9-C4-C5	5.44	107.98	105.80
33	BA	2187	A	C4-C5-C6	5.44	119.72	117.00
33	BA	2722	A	C4-C5-N7	-5.44	107.98	110.70
34	BB	44	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	296	A	N9-C4-C5	5.44	107.98	105.80
1	AA	956	A	N9-C4-C5	5.44	107.98	105.80
1	AA	1121	A	N9-C4-C5	5.44	107.98	105.80
33	BA	176	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	786	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	1818	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	2455	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	2807	A	C4-C5-C6	5.44	119.72	117.00
34	BB	97	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	390	A	N9-C4-C5	5.44	107.98	105.80
1	AA	831	A	N9-C4-C5	5.44	107.98	105.80
1	AA	1092	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	1427	A	N9-C4-C5	5.44	107.98	105.80
33	BA	139	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	202	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	421	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	160	A	N9-C4-C5	5.44	107.97	105.80
1	AA	485	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	529	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	1180	A	N9-C4-C5	5.44	107.97	105.80
1	AA	1463	A	C8-N9-C4	5.44	107.97	105.80
33	BA	5	A	N9-C4-C5	5.44	107.97	105.80
33	BA	199	A	N9-C4-C5	5.44	107.97	105.80
33	BA	225	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	428	A	N9-C4-C5	5.44	107.97	105.80
33	BA	1025	A	C8-N9-C4	5.44	107.97	105.80
33	BA	1375	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	1392	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	1929	A	N9-C4-C5	5.44	107.97	105.80
33	BA	2047	A	C4-C5-N7	-5.44	107.98	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2440	A	N9-C4-C5	5.44	107.97	105.80
33	BA	2661	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	2668	A	N9-C4-C5	5.44	107.97	105.80
33	BA	2686	A	C4-C5-N7	-5.44	107.98	110.70
33	BA	2704	A	N9-C4-C5	5.44	107.97	105.80
33	BA	2807	A	N3-C4-N9	5.44	131.75	127.40
34	BB	114	A	N9-C4-C5	5.44	107.97	105.80
1	AA	1048	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	1252	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	1298	A	C4-C5-N7	-5.44	107.98	110.70
21	AX	44	A	N9-C4-C5	5.44	107.97	105.80
33	BA	229	A	N9-C4-C5	5.44	107.97	105.80
33	BA	1260	A	C8-N9-C4	5.44	107.97	105.80
33	BA	1814	A	C8-N9-C4	5.44	107.97	105.80
33	BA	2165	A	N9-C4-C5	5.44	107.97	105.80
33	BA	2187	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	203	A	N9-C4-C5	5.43	107.97	105.80
1	AA	323	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	364	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	389	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	438	A	N9-C4-C5	5.43	107.97	105.80
1	AA	979	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	1017	A	C8-N9-C4	5.43	107.97	105.80
1	AA	1166	A	C5-C6-N1	5.43	120.42	117.70
33	BA	126	A	N9-C4-C5	5.43	107.97	105.80
33	BA	162	A	N9-C4-C5	5.43	107.97	105.80
33	BA	219	A	N9-C4-C5	5.43	107.97	105.80
33	BA	1020	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	1335	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	2777	A	N9-C4-C5	5.43	107.97	105.80
1	AA	52	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	67	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	463	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	831	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	1006	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	1103	A	N9-C4-C5	5.43	107.97	105.80
1	AA	1260	A	N9-C4-C5	5.43	107.97	105.80
33	BA	198	A	N9-C4-C5	5.43	107.97	105.80
33	BA	553	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	758	A	N9-C4-C5	5.43	107.97	105.80
33	BA	762	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	1096	A	C4-C5-N7	-5.43	107.98	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1724	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	2303	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	2406	A	N9-C4-C5	5.43	107.97	105.80
33	BA	2643	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	2876	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	195	A	C5-C6-N1	5.43	120.42	117.70
1	AA	664	A	N9-C4-C5	5.43	107.97	105.80
1	AA	945	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	1490	A	C8-N9-C4	5.43	107.97	105.80
33	BA	2302	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	2804	A	C8-N9-C4	5.43	107.97	105.80
1	AA	910	A	C4-C5-N7	-5.43	107.98	110.70
1	AA	974	A	N9-C4-C5	5.43	107.97	105.80
21	AX	14	A	N9-C4-C5	5.43	107.97	105.80
33	BA	519	A	N9-C4-C5	5.43	107.97	105.80
33	BA	851	A	C8-N9-C4	5.43	107.97	105.80
33	BA	1072	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	1406	A	C4-C5-N7	-5.43	107.98	110.70
33	BA	2228	A	C8-N9-C4	5.43	107.97	105.80
33	BA	2417	A	N9-C4-C5	5.43	107.97	105.80
1	AA	18	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	439	A	C4-C5-C6	5.43	119.71	117.00
1	AA	519	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	685	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	1435	A	C8-N9-C4	5.43	107.97	105.80
33	BA	904	A	C8-N9-C4	5.43	107.97	105.80
33	BA	1735	A	N9-C4-C5	5.43	107.97	105.80
33	BA	1789	A	C4-C5-N7	-5.43	107.99	110.70
33	BA	2146	A	C8-N9-C4	5.43	107.97	105.80
33	BA	2482	A	N9-C4-C5	5.43	107.97	105.80
33	BA	2590	A	N9-C4-C5	5.43	107.97	105.80
33	BA	2893	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	28	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	582	A	C8-N9-C4	5.43	107.97	105.80
1	AA	679	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	1451	A	C4-C5-N7	-5.43	107.99	110.70
33	BA	10	A	C8-N9-C4	5.43	107.97	105.80
33	BA	273	A	C8-N9-C4	5.43	107.97	105.80
33	BA	582	A	N9-C4-C5	5.43	107.97	105.80
33	BA	821	A	N9-C4-C5	5.43	107.97	105.80
33	BA	828	A	C4-C5-N7	-5.43	107.99	110.70
33	BA	894	A	C4-C5-N7	-5.43	107.99	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1844	A	C4-C5-C6	5.43	119.71	117.00
33	BA	1941	A	N3-C4-N9	5.43	131.74	127.40
33	BA	2819	A	N9-C4-C5	5.43	107.97	105.80
33	BA	2875	A	N9-C4-C5	5.43	107.97	105.80
33	BA	2900	A	C4-C5-N7	-5.43	107.99	110.70
34	BB	13	A	C8-N9-C4	5.43	107.97	105.80
34	BB	105	A	C4-C5-N7	-5.43	107.99	110.70
1	AA	206	A	N9-C4-C5	5.42	107.97	105.80
1	AA	404	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	568	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	870	A	C8-N9-C4	5.42	107.97	105.80
1	AA	902	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	947	A	N9-C4-C5	5.42	107.97	105.80
1	AA	1200	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	1359	A	N9-C4-C5	5.42	107.97	105.80
1	AA	1383	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	1512	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	73	A	C8-N9-C4	5.42	107.97	105.80
33	BA	330	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	456	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	943	A	C8-N9-C4	5.42	107.97	105.80
33	BA	1617	A	N9-C4-C5	5.42	107.97	105.80
33	BA	1721	A	C8-N9-C4	5.42	107.97	105.80
33	BA	1791	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1882	A	N9-C4-C5	5.42	107.97	105.80
33	BA	2507	A	N9-C4-C5	5.42	107.97	105.80
33	BA	2542	A	C4-C5-N7	-5.42	107.99	110.70
34	BB	37	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	228	A	N9-C4-C5	5.42	107.97	105.80
1	AA	459	A	C8-N9-C4	5.42	107.97	105.80
1	AA	459	A	N9-C4-C5	5.42	107.97	105.80
33	BA	448	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	746	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1059	A	N9-C4-C5	5.42	107.97	105.80
33	BA	2830	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	52	A	N9-C4-C5	5.42	107.97	105.80
1	AA	371	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	397	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	457	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	542	A	N9-C4-C5	5.42	107.97	105.80
1	AA	544	A	N9-C4-C5	5.42	107.97	105.80
1	AA	837	A	C4-C5-N7	-5.42	107.99	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	985	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	1065	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	1128	A	N9-C4-C5	5.42	107.97	105.80
21	AX	21	A	N9-C4-C5	5.42	107.97	105.80
33	BA	1036	A	N9-C4-C5	5.42	107.97	105.80
33	BA	1381	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1456	A	C8-N9-C4	5.42	107.97	105.80
33	BA	1745	A	C8-N9-C4	5.42	107.97	105.80
33	BA	1877	A	N9-C4-C5	5.42	107.97	105.80
33	BA	1882	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	2406	A	C8-N9-C4	5.42	107.97	105.80
33	BA	2497	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	2511	A	C8-N9-C4	5.42	107.97	105.80
33	BA	2770	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	2845	A	C8-N9-C4	5.42	107.97	105.80
1	AA	459	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	638	A	N9-C4-C5	5.42	107.97	105.80
1	AA	825	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	1031	A	C8-N9-C4	5.42	107.97	105.80
33	BA	904	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1579	A	C8-N9-C4	5.42	107.97	105.80
33	BA	1850	A	C8-N9-C4	5.42	107.97	105.80
33	BA	2100	A	C8-N9-C4	5.42	107.97	105.80
1	AA	53	A	N9-C4-C5	5.42	107.97	105.80
1	AA	55	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	74	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	234	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	704	A	N9-C4-C5	5.42	107.97	105.80
1	AA	768	A	N9-C4-C5	5.42	107.97	105.80
1	AA	862	A	C4-C5-C6	5.42	119.71	117.00
1	AA	1024	A	C8-N9-C4	5.42	107.97	105.80
33	BA	65	A	N9-C4-C5	5.42	107.97	105.80
33	BA	326	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	436	A	N9-C4-C5	5.42	107.97	105.80
33	BA	917	A	N9-C4-C5	5.42	107.97	105.80
33	BA	1388	A	C8-N9-C4	5.42	107.97	105.80
33	BA	1398	A	C8-N9-C4	5.42	107.97	105.80
33	BA	1947	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	2060	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	2087	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	2480	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	209	A	C8-N9-C4	5.42	107.97	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AX	23	A	C8-N9-C4	5.42	107.97	105.80
33	BA	194	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1027	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1092	A	C8-N9-C4	5.42	107.97	105.80
33	BA	1113	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1406	A	N9-C4-C5	5.42	107.97	105.80
33	BA	1663	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1844	A	N3-C4-N9	5.42	131.73	127.40
33	BA	1876	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1928	A	N9-C4-C5	5.42	107.97	105.80
33	BA	2330	A	C8-N9-C4	5.42	107.97	105.80
33	BA	2340	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	2351	A	C8-N9-C4	5.42	107.97	105.80
1	AA	923	A	N9-C4-C5	5.42	107.97	105.80
1	AA	1284	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	373	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1412	A	N9-C4-C5	5.42	107.97	105.80
33	BA	1556	A	C4-C5-N7	-5.42	107.99	110.70
33	BA	1948	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	270	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	496	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	504	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	685	A	N9-C4-C5	5.41	107.97	105.80
1	AA	979	A	N9-C4-C5	5.41	107.97	105.80
1	AA	1102	A	C4-C5-N7	-5.41	107.99	110.70
33	BA	125	A	C8-N9-C4	5.41	107.97	105.80
33	BA	126	A	C4-C5-N7	-5.41	107.99	110.70
33	BA	144	A	C4-C5-N7	-5.41	107.99	110.70
33	BA	200	A	C4-C5-N7	-5.41	107.99	110.70
33	BA	494	A	N3-C4-N9	5.41	131.73	127.40
33	BA	530	A	C4-C5-N7	-5.41	107.99	110.70
33	BA	646	A	N9-C4-C5	5.41	107.97	105.80
33	BA	1532	A	C4-C5-N7	-5.41	107.99	110.70
33	BA	2327	A	N9-C4-C5	5.41	107.97	105.80
33	BA	2785	U	P-O3'-C3'	5.41	126.20	119.70
33	BA	2810	A	C4-C5-N7	-5.41	107.99	110.70
34	BB	11	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	371	A	N9-C4-C5	5.41	107.97	105.80
1	AA	724	A	C8-N9-C4	5.41	107.97	105.80
33	BA	64	A	C4-C5-N7	-5.41	107.99	110.70
33	BA	504	A	N3-C4-N9	5.41	131.73	127.40
33	BA	1465	A	C4-C5-N7	-5.41	107.99	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1941	A	C8-N9-C4	5.41	107.97	105.80
1	AA	204	A	N9-C4-C5	5.41	107.96	105.80
1	AA	485	A	N9-C4-C5	5.41	107.96	105.80
1	AA	671	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1327	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1333	A	C8-N9-C4	5.41	107.96	105.80
1	AA	1348	A	C4-C5-N7	-5.41	107.99	110.70
33	BA	53	A	N9-C4-C5	5.41	107.96	105.80
33	BA	265	A	C8-N9-C4	5.41	107.96	105.80
33	BA	574	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	849	A	N9-C4-C5	5.41	107.97	105.80
33	BA	851	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	1123	A	N9-C4-C5	5.41	107.96	105.80
33	BA	1224	A	N9-C4-C5	5.41	107.97	105.80
33	BA	1340	A	C4-C5-C6	5.41	119.70	117.00
33	BA	1882	A	C8-N9-C4	5.41	107.96	105.80
33	BA	2560	A	C4-C5-N7	-5.41	107.99	110.70
1	AA	352	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	616	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	737	A	C8-N9-C4	5.41	107.96	105.80
1	AA	1407	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1512	A	N9-C4-C5	5.41	107.96	105.80
33	BA	384	A	C8-N9-C4	5.41	107.96	105.80
33	BA	653	A	N9-C4-C5	5.41	107.96	105.80
33	BA	705	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	867	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	1254	A	N9-C4-C5	5.41	107.96	105.80
33	BA	1269	A	N9-C4-C5	5.41	107.96	105.80
33	BA	1848	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	1918	A	N9-C4-C5	5.41	107.96	105.80
33	BA	2594	A	N9-C4-C5	5.41	107.96	105.80
34	BB	102	A	C8-N9-C4	5.41	107.96	105.80
1	AA	161	A	C8-N9-C4	5.41	107.96	105.80
1	AA	583	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	630	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	651	A	N9-C4-C5	5.41	107.96	105.80
1	AA	757	A	N9-C4-C5	5.41	107.96	105.80
1	AA	799	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1259	A	N9-C4-C5	5.41	107.96	105.80
1	AA	1369	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1470	A	N9-C4-C5	5.41	107.96	105.80
33	BA	206	A	C8-N9-C4	5.41	107.96	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	547	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	1760	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	1989	A	N9-C4-C5	5.41	107.96	105.80
33	BA	2500	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	2590	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	170	A	C8-N9-C4	5.41	107.96	105.80
1	AA	811	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	948	A	C8-N9-C4	5.41	107.96	105.80
1	AA	1014	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1197	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	1289	A	N9-C4-C5	5.41	107.96	105.80
1	AA	1358	A	N9-C4-C5	5.41	107.96	105.80
33	BA	236	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	592	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	1008	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	1357	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	1473	A	N3-C4-N9	5.41	131.72	127.40
33	BA	1580	A	N9-C4-C5	5.41	107.96	105.80
33	BA	1743	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	2088	A	N9-C4-C5	5.41	107.96	105.80
33	BA	2187	A	N9-C4-C5	5.41	107.96	105.80
33	BA	2421	A	C4-C5-N7	-5.41	108.00	110.70
33	BA	2854	A	N9-C4-C5	5.41	107.96	105.80
1	AA	209	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	674	A	N3-C4-N9	5.40	131.72	127.40
1	AA	796	A	N9-C4-C5	5.40	107.96	105.80
21	AX	24	A	C8-N9-C4	5.40	107.96	105.80
33	BA	168	A	C8-N9-C4	5.40	107.96	105.80
33	BA	198	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	429	A	N9-C4-C5	5.40	107.96	105.80
33	BA	1126	A	C5-C6-N1	5.40	120.40	117.70
33	BA	1326	A	N9-C4-C5	5.40	107.96	105.80
33	BA	1850	A	N9-C4-C5	5.40	107.96	105.80
34	BB	44	A	N9-C4-C5	5.40	107.96	105.80
1	AA	314	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	462	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	631	A	C8-N9-C4	5.40	107.96	105.80
1	AA	1236	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	94	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	329	A	N9-C4-C5	5.40	107.96	105.80
33	BA	333	A	N9-C4-C5	5.40	107.96	105.80
33	BA	584	A	N9-C4-C5	5.40	107.96	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1094	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	1132	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	1421	A	C8-N9-C4	5.40	107.96	105.80
33	BA	1967	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	2078	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	2106	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	2351	A	N9-C4-C5	5.40	107.96	105.80
33	BA	2769	A	C8-N9-C4	5.40	107.96	105.80
34	BB	105	A	N9-C4-C5	5.40	107.96	105.80
1	AA	129	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	364	A	N9-C4-C5	5.40	107.96	105.80
1	AA	1261	A	N9-C4-C5	5.40	107.96	105.80
1	AA	1435	A	N9-C4-C5	5.40	107.96	105.80
33	BA	448	A	N9-C4-C5	5.40	107.96	105.80
33	BA	781	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	1113	A	N9-C4-C5	5.40	107.96	105.80
33	BA	1286	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	1791	A	C8-N9-C4	5.40	107.96	105.80
33	BA	1981	A	C8-N9-C4	5.40	107.96	105.80
33	BA	2369	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	618	A	N9-C4-C5	5.40	107.96	105.80
1	AA	1179	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	1486	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	329	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	2256	A	N9-C4-C5	5.40	107.96	105.80
1	AA	282	A	N9-C4-C5	5.40	107.96	105.80
1	AA	703	A	N9-C4-C5	5.40	107.96	105.80
33	BA	355	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	1685	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	1838	A	C8-N9-C4	5.40	107.96	105.80
34	BB	56	A	N9-C4-C5	5.40	107.96	105.80
1	AA	474	A	N9-C4-C5	5.40	107.96	105.80
1	AA	715	A	C8-N9-C4	5.40	107.96	105.80
21	AX	70	A	C8-N9-C4	5.40	107.96	105.80
33	BA	94	A	N9-C4-C5	5.40	107.96	105.80
33	BA	677	A	N9-C4-C5	5.40	107.96	105.80
33	BA	1680	A	C8-N9-C4	5.40	107.96	105.80
33	BA	2254	A	C4-C5-C6	5.40	119.70	117.00
33	BA	2387	A	N9-C4-C5	5.40	107.96	105.80
33	BA	2658	A	N9-C4-C5	5.40	107.96	105.80
33	BA	2826	A	C4-C5-N7	-5.40	108.00	110.70
33	BA	2860	A	C4-C5-N7	-5.40	108.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	969	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	1054	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	14	A	C8-N9-C4	5.39	107.96	105.80
33	BA	1003	A	N3-C4-N9	5.39	131.72	127.40
33	BA	1445	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	1788	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	1885	A	N9-C4-C5	5.39	107.96	105.80
33	BA	2000	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	2616	A	N9-C4-C5	5.39	107.96	105.80
1	AA	120	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	220	A	C8-N9-C4	5.39	107.96	105.80
33	BA	1313	A	N9-C4-C5	5.39	107.96	105.80
33	BA	1517	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	1929	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	1930	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	2461	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	2595	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	711	A	C8-N9-C4	5.39	107.96	105.80
1	AA	1341	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	28	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	265	A	N9-C4-C5	5.39	107.96	105.80
33	BA	388	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	702	A	N9-C4-C5	5.39	107.96	105.80
33	BA	1020	A	N9-C4-C5	5.39	107.96	105.80
1	AA	62	A	N9-C4-C5	5.39	107.96	105.80
1	AA	776	A	N9-C4-C5	5.39	107.96	105.80
1	AA	1120	A	N9-C4-C5	5.39	107.95	105.80
1	AA	1270	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	1403	A	N9-C4-C5	5.39	107.96	105.80
1	AA	1466	A	N9-C4-C5	5.39	107.96	105.80
33	BA	343	A	C4-C5-N7	-5.39	108.00	110.70
33	BA	630	A	C8-N9-C4	5.39	107.96	105.80
33	BA	1056	A	C4-C5-N7	-5.39	108.01	110.70
33	BA	1096	A	N9-C4-C5	5.39	107.96	105.80
33	BA	1713	A	N9-C4-C5	5.39	107.96	105.80
33	BA	2329	A	C4-C5-N7	-5.39	108.01	110.70
33	BA	2869	A	C8-N9-C4	5.39	107.96	105.80
34	BB	113	A	C4-C5-N7	-5.39	108.01	110.70
1	AA	118	A	C4-C5-N7	-5.39	108.01	110.70
1	AA	1048	A	N9-C4-C5	5.39	107.95	105.80
33	BA	1026	A	N9-C4-C5	5.39	107.95	105.80
33	BA	2511	A	N9-C4-C5	5.39	107.95	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	55	A	N9-C4-C5	5.39	107.95	105.80
33	BA	65	A	C4-C5-N7	-5.39	108.01	110.70
33	BA	524	A	C4-C5-N7	-5.39	108.01	110.70
33	BA	678	A	C4-C5-N7	-5.39	108.01	110.70
33	BA	1490	A	C4-C5-N7	-5.39	108.01	110.70
33	BA	1579	A	C4-C5-N7	-5.39	108.01	110.70
33	BA	1710	A	C8-N9-C4	5.39	107.95	105.80
33	BA	1767	A	C4-C5-N7	-5.39	108.01	110.70
33	BA	2316	A	C4-C5-N7	-5.39	108.01	110.70
33	BA	2338	A	N9-C4-C5	5.39	107.95	105.80
33	BA	2919	A	C4-C5-N7	-5.39	108.01	110.70
34	BB	50	A	N9-C4-C5	5.39	107.95	105.80
1	AA	423	A	N9-C4-C5	5.38	107.95	105.80
33	BA	259	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	449	A	N9-C4-C5	5.38	107.95	105.80
33	BA	476	A	C8-N9-C4	5.38	107.95	105.80
33	BA	494	A	C4-C5-C6	5.38	119.69	117.00
33	BA	782	A	N9-C4-C5	5.38	107.95	105.80
33	BA	896	A	C8-N9-C4	5.38	107.95	105.80
33	BA	1097	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1235	A	C8-N9-C4	5.38	107.95	105.80
33	BA	1601	A	C8-N9-C4	5.38	107.95	105.80
33	BA	1699	A	N9-C4-C5	5.38	107.95	105.80
33	BA	1760	A	N9-C4-C5	5.38	107.95	105.80
33	BA	2034	A	N9-C4-C5	5.38	107.95	105.80
33	BA	2060	A	C8-N9-C4	5.38	107.95	105.80
33	BA	2087	A	N9-C4-C5	5.38	107.95	105.80
33	BA	2132	A	N9-C4-C5	5.38	107.95	105.80
33	BA	2740	A	N9-C4-C5	5.38	107.95	105.80
33	BA	2912	A	C4-C5-N7	-5.38	108.01	110.70
34	BB	11	A	N9-C4-C5	5.38	107.95	105.80
1	AA	475	A	C8-N9-C4	5.38	107.95	105.80
33	BA	354	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	561	A	N9-C4-C5	5.38	107.95	105.80
33	BA	1542	A	C8-N9-C4	5.38	107.95	105.80
33	BA	2007	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	2526	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	2560	A	C8-N9-C4	5.38	107.95	105.80
1	AA	72	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	150	A	N3-C4-N9	5.38	131.71	127.40
1	AA	382	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	844	A	C8-N9-C4	5.38	107.95	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1077	A	N9-C4-C5	5.38	107.95	105.80
1	AA	1509	A	N9-C4-C5	5.38	107.95	105.80
33	BA	90	A	C8-N9-C4	5.38	107.95	105.80
33	BA	469	A	N9-C4-C5	5.38	107.95	105.80
33	BA	561	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1116	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1388	A	N9-C4-C5	5.38	107.95	105.80
33	BA	1663	A	N9-C4-C5	5.38	107.95	105.80
33	BA	1713	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	2111	A	C8-N9-C4	5.38	107.95	105.80
33	BA	2482	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	555	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1176	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1427	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	437	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1743	A	N9-C4-C5	5.38	107.95	105.80
33	BA	2000	A	N9-C4-C5	5.38	107.95	105.80
33	BA	2497	A	N9-C4-C5	5.38	107.95	105.80
33	BA	2793	A	N3-C4-N9	5.38	131.70	127.40
33	BA	2898	A	N3-C4-N9	5.38	131.70	127.40
33	BA	889	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	974	A	N9-C4-C5	5.38	107.95	105.80
33	BA	1188	A	C4-C5-C6	5.38	119.69	117.00
33	BA	1361	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1432	A	N9-C4-C5	5.38	107.95	105.80
33	BA	1506	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1541	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1556	A	N9-C4-C5	5.38	107.95	105.80
33	BA	1710	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1767	A	C8-N9-C4	5.38	107.95	105.80
33	BA	1999	A	C8-N9-C4	5.38	107.95	105.80
33	BA	2497	A	C8-N9-C4	5.38	107.95	105.80
33	BA	2704	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	2827	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	771	A	N9-C4-C5	5.38	107.95	105.80
1	AA	1031	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1205	A	N9-C4-C5	5.38	107.95	105.80
1	AA	1455	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	91	A	C8-N9-C4	5.38	107.95	105.80
33	BA	102	A	N9-C4-C5	5.38	107.95	105.80
33	BA	390	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1421	A	N9-C4-C5	5.38	107.95	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1553	A	N9-C4-C5	5.38	107.95	105.80
33	BA	1555	A	C4-C5-C6	5.38	119.69	117.00
33	BA	2083	A	N9-C4-C5	5.38	107.95	105.80
33	BA	2793	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	372	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	713	A	C4-C5-C6	5.38	119.69	117.00
33	BA	247	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	753	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1453	A	C4-C5-N7	-5.38	108.01	110.70
33	BA	1569	A	C4-C5-N7	-5.38	108.01	110.70
34	BB	71	A	C8-N9-C4	5.38	107.95	105.80
1	AA	389	A	N9-C4-C5	5.37	107.95	105.80
1	AA	415	A	N9-C4-C5	5.37	107.95	105.80
1	AA	433	A	C4-C5-N7	-5.37	108.01	110.70
1	AA	945	A	N9-C4-C5	5.37	107.95	105.80
1	AA	1024	A	N9-C4-C5	5.37	107.95	105.80
1	AA	1261	A	C8-N9-C4	5.37	107.95	105.80
1	AA	1455	A	N9-C4-C5	5.37	107.95	105.80
33	BA	13	A	C4-C5-N7	-5.37	108.01	110.70
33	BA	619	A	C4-C5-N7	-5.37	108.01	110.70
33	BA	1608	A	C4-C5-N7	-5.37	108.01	110.70
33	BA	2119	A	N9-C4-C5	5.37	107.95	105.80
33	BA	2298	A	N9-C4-C5	5.37	107.95	105.80
33	BA	2440	A	C8-N9-C4	5.37	107.95	105.80
33	BA	2547	A	C4-C5-N7	-5.37	108.01	110.70
33	BA	2694	A	C4-C5-N7	-5.37	108.01	110.70
1	AA	352	A	N9-C4-C5	5.37	107.95	105.80
1	AA	372	A	N9-C4-C5	5.37	107.95	105.80
1	AA	491	A	N9-C4-C5	5.37	107.95	105.80
33	BA	437	A	N9-C4-C5	5.37	107.95	105.80
33	BA	896	A	C4-C5-N7	-5.37	108.01	110.70
33	BA	1312	A	N9-C4-C5	5.37	107.95	105.80
1	AA	463	A	N9-C4-C5	5.37	107.95	105.80
1	AA	1222	A	N9-C4-C5	5.37	107.95	105.80
33	BA	326	A	N9-C4-C5	5.37	107.95	105.80
33	BA	353	A	C8-N9-C4	5.37	107.95	105.80
33	BA	1029	A	C8-N9-C4	5.37	107.95	105.80
33	BA	1265	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	1845	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	2440	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	2606	A	N3-C4-N9	5.37	131.70	127.40
1	AA	211	A	C4-C5-N7	-5.37	108.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	604	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	918	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	1200	A	N9-C4-C5	5.37	107.95	105.80
33	BA	199	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	475	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	547	A	N9-C4-C5	5.37	107.95	105.80
33	BA	1073	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	1723	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	2078	A	N9-C4-C5	5.37	107.95	105.80
33	BA	2155	A	N9-C4-C5	5.37	107.95	105.80
33	BA	2461	A	N9-C4-C5	5.37	107.95	105.80
33	BA	2526	A	N9-C4-C5	5.37	107.95	105.80
33	BA	2670	A	N3-C4-N9	5.37	131.69	127.40
33	BA	2924	A	N9-C4-C5	5.37	107.95	105.80
1	AA	1328	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	727	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	786	A	N9-C4-C5	5.37	107.95	105.80
33	BA	1421	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	35	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	474	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	793	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	824	A	N9-C4-C5	5.37	107.95	105.80
1	AA	1054	A	N9-C4-C5	5.37	107.95	105.80
1	AA	1349	A	N9-C4-C5	5.37	107.95	105.80
21	AX	58	A	N9-C4-C5	5.37	107.95	105.80
33	BA	38	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	324	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	339	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	746	A	N9-C4-C5	5.37	107.95	105.80
33	BA	867	A	C8-N9-C4	5.37	107.95	105.80
33	BA	1308	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	1405	A	N9-C4-C5	5.37	107.95	105.80
33	BA	1723	A	N9-C4-C5	5.37	107.95	105.80
33	BA	2042	A	C4-C5-N7	-5.37	108.02	110.70
33	BA	2047	A	N9-C4-C5	5.37	107.95	105.80
33	BA	2389	A	N9-C4-C5	5.37	107.95	105.80
33	BA	2542	A	N9-C4-C5	5.37	107.95	105.80
1	AA	67	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1031	A	N9-C4-C5	5.36	107.95	105.80
1	AA	1298	A	N9-C4-C5	5.36	107.95	105.80
1	AA	1366	A	C8-N9-C4	5.36	107.95	105.80
1	AA	1479	A	C4-C5-N7	-5.36	108.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1529	A	N9-C4-C5	5.36	107.94	105.80
33	BA	185	A	C8-N9-C4	5.36	107.94	105.80
33	BA	1532	A	N9-C4-C5	5.36	107.95	105.80
33	BA	1541	A	N9-C4-C5	5.36	107.95	105.80
33	BA	2848	A	N9-C4-C5	5.36	107.95	105.80
1	AA	1189	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1490	A	C4-C5-N7	-5.36	108.02	110.70
21	AX	70	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	216	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	490	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	236	A	N9-C4-C5	5.36	107.94	105.80
1	AA	270	A	N9-C4-C5	5.36	107.94	105.80
1	AA	271	A	C8-N9-C4	5.36	107.94	105.80
1	AA	512	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	529	A	N9-C4-C5	5.36	107.94	105.80
33	BA	110	A	N9-C4-C5	5.36	107.94	105.80
33	BA	185	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	225	A	N9-C4-C5	5.36	107.94	105.80
33	BA	1221	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	1233	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	1982	A	N3-C4-N9	5.36	131.69	127.40
33	BA	2343	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	2734	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	404	A	N9-C4-C5	5.36	107.94	105.80
1	AA	705	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	507	A	N9-C4-C5	5.36	107.94	105.80
33	BA	769	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	910	A	C5-C6-N1	5.36	120.38	117.70
33	BA	2042	A	N9-C4-C5	5.36	107.94	105.80
1	AA	94	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	173	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1210	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1271	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1342	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	162	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	200	A	N9-C4-C5	5.36	107.94	105.80
33	BA	1388	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	1619	A	C8-N9-C4	5.36	107.94	105.80
33	BA	2389	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	2405	A	C8-N9-C4	5.36	107.94	105.80
33	BA	2889	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	2924	A	C4-C5-N7	-5.36	108.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	984	A	C8-N9-C4	5.36	107.94	105.80
1	AA	1185	A	N9-C4-C5	5.36	107.94	105.80
21	AX	41	A	N9-C4-C5	5.36	107.94	105.80
33	BA	38	A	N9-C4-C5	5.36	107.94	105.80
33	BA	849	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	1073	A	C8-N9-C4	5.36	107.94	105.80
33	BA	1323	A	N9-C4-C5	5.36	107.94	105.80
33	BA	1426	A	C4-C5-N7	-5.36	108.02	110.70
33	BA	2661	A	N9-C4-C5	5.36	107.94	105.80
34	BB	50	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	333	A	N9-C4-C5	5.35	107.94	105.80
1	AA	988	A	N3-C4-N9	5.35	131.68	127.40
1	AA	1024	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	1225	A	N9-C4-C5	5.35	107.94	105.80
33	BA	369	A	C4-C5-N7	-5.35	108.02	110.70
33	BA	600	A	N9-C4-C5	5.35	107.94	105.80
33	BA	1266	A	C8-N9-C4	5.35	107.94	105.80
33	BA	1445	A	N9-C4-C5	5.35	107.94	105.80
33	BA	1506	A	N9-C4-C5	5.35	107.94	105.80
34	BB	51	A	C4-C5-N7	-5.35	108.02	110.70
33	BA	318	A	C4-C5-N7	-5.35	108.03	110.70
33	BA	412	A	N9-C4-C5	5.35	107.94	105.80
33	BA	868	A	C4-C5-N7	-5.35	108.03	110.70
33	BA	1464	A	N9-C4-C5	5.35	107.94	105.80
33	BA	2517	A	C8-N9-C4	5.35	107.94	105.80
33	BA	2912	A	N9-C4-C5	5.35	107.94	105.80
1	AA	151	A	N3-C4-N9	5.35	131.68	127.40
1	AA	1189	A	C4-C5-N7	-5.35	108.03	110.70
1	AA	1479	A	N9-C4-C5	5.35	107.94	105.80
33	BA	896	A	N9-C4-C5	5.35	107.94	105.80
33	BA	1036	A	C4-C5-N7	-5.35	108.03	110.70
33	BA	1533	A	N9-C4-C5	5.35	107.94	105.80
33	BA	1877	A	C4-C5-N7	-5.35	108.03	110.70
33	BA	1942	A	N9-C4-C5	5.35	107.94	105.80
33	BA	2477	A	N9-C4-C5	5.35	107.94	105.80
33	BA	2787	A	C4-C5-N7	-5.35	108.03	110.70
33	BA	2834	A	C8-N9-C4	5.35	107.94	105.80
1	AA	34	A	N9-C4-C5	5.35	107.94	105.80
1	AA	34	A	C4-C5-N7	-5.35	108.03	110.70
1	AA	290	A	N9-C4-C5	5.35	107.94	105.80
1	AA	611	A	C4-C5-N7	-5.35	108.03	110.70
1	AA	762	A	N9-C4-C5	5.35	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1128	A	C4-C5-N7	-5.35	108.03	110.70
33	BA	325	A	N9-C4-C5	5.35	107.94	105.80
33	BA	913	A	C8-N9-C4	5.35	107.94	105.80
33	BA	1074	A	C4-C5-N7	-5.35	108.03	110.70
33	BA	1734	A	N9-C4-C5	5.35	107.94	105.80
33	BA	1767	A	N9-C4-C5	5.35	107.94	105.80
33	BA	2722	A	N9-C4-C5	5.35	107.94	105.80
33	BA	139	A	N9-C4-C5	5.35	107.94	105.80
33	BA	1722	A	C4-C5-N7	-5.35	108.03	110.70
1	AA	793	A	N9-C4-C5	5.34	107.94	105.80
1	AA	883	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	1342	A	N9-C4-C5	5.34	107.94	105.80
33	BA	1116	A	N9-C4-C5	5.34	107.94	105.80
33	BA	1710	A	N9-C4-C5	5.34	107.94	105.80
33	BA	2517	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1102	A	N9-C4-C5	5.34	107.94	105.80
33	BA	407	A	C8-N9-C4	5.34	107.94	105.80
33	BA	592	A	N9-C4-C5	5.34	107.94	105.80
33	BA	593	A	C4-C5-N7	-5.34	108.03	110.70
33	BA	769	A	N9-C4-C5	5.34	107.94	105.80
33	BA	1361	A	N9-C4-C5	5.34	107.94	105.80
33	BA	1424	A	C4-C5-N7	-5.34	108.03	110.70
33	BA	2276	A	N9-C4-C5	5.34	107.94	105.80
1	AA	74	A	N9-C4-C5	5.34	107.94	105.80
1	AA	491	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	828	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1155	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1283	A	C8-N9-C4	5.34	107.94	105.80
1	AA	1315	A	C4-C5-N7	-5.34	108.03	110.70
33	BA	259	A	N9-C4-C5	5.34	107.94	105.80
33	BA	517	A	C4-C5-N7	-5.34	108.03	110.70
33	BA	578	A	C4-C5-N7	-5.34	108.03	110.70
33	BA	1619	A	C4-C5-N7	-5.34	108.03	110.70
33	BA	1675	A	N9-C4-C5	5.34	107.94	105.80
33	BA	1850	A	C4-C5-N7	-5.34	108.03	110.70
33	BA	2704	A	C8-N9-C4	5.34	107.94	105.80
33	BA	2876	A	N9-C4-C5	5.34	107.94	105.80
34	BB	76	A	N9-C4-C5	5.34	107.94	105.80
1	AA	61	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	438	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	649	A	C5-C6-N1	5.34	120.37	117.70
1	AA	659	A	C4-C5-N7	-5.34	108.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1308	A	C5-C6-N1	5.34	120.37	117.70
33	BA	1201	A	C4-C5-C6	5.34	119.67	117.00
33	BA	1556	A	C8-N9-C4	5.34	107.94	105.80
33	BA	2619	A	C4-C5-N7	-5.34	108.03	110.70
33	BA	2708	A	C4-C5-N7	-5.34	108.03	110.70
34	BB	71	A	C4-C5-N7	-5.34	108.03	110.70
34	BB	113	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1248	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1252	A	N9-C4-C5	5.34	107.94	105.80
21	AX	23	A	C4-C5-N7	-5.34	108.03	110.70
33	BA	876	A	N9-C4-C5	5.34	107.94	105.80
33	BA	958	A	C8-N9-C4	5.34	107.94	105.80
33	BA	2297	A	N9-C4-C5	5.34	107.94	105.80
1	AA	386	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1486	A	N9-C4-C5	5.34	107.94	105.80
33	BA	91	A	C4-C5-N7	-5.34	108.03	110.70
33	BA	496	A	C8-N9-C4	5.34	107.93	105.80
33	BA	781	A	N9-C4-C5	5.34	107.94	105.80
33	BA	2123	A	C5-C6-N1	5.34	120.37	117.70
33	BA	2826	A	N9-C4-C5	5.34	107.94	105.80
1	AA	290	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	1160	A	C4-C5-N7	-5.33	108.03	110.70
33	BA	829	A	N9-C4-C5	5.33	107.93	105.80
33	BA	1504	A	N9-C4-C5	5.33	107.93	105.80
33	BA	1774	A	N9-C4-C5	5.33	107.93	105.80
33	BA	2848	A	C8-N9-C4	5.33	107.93	105.80
1	AA	1056	A	N9-C4-C5	5.33	107.93	105.80
1	AA	1092	A	N9-C4-C5	5.33	107.93	105.80
21	AX	9	A	C8-N9-C4	5.33	107.93	105.80
33	BA	1540	A	N9-C4-C5	5.33	107.93	105.80
33	BA	2875	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	173	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	696	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	968	A	C8-N9-C4	5.33	107.93	105.80
33	BA	438	A	C4-C5-N7	-5.33	108.03	110.70
33	BA	1075	A	C4-C5-N7	-5.33	108.03	110.70
33	BA	1393	A	C8-N9-C4	5.33	107.93	105.80
33	BA	2778	A	C4-C5-N7	-5.33	108.03	110.70
33	BA	376	A	N9-C4-C5	5.33	107.93	105.80
33	BA	1453	A	N9-C4-C5	5.33	107.93	105.80
33	BA	2043	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	55	A	N9-C4-C5	5.33	107.93	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	140	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	314	A	N9-C4-C5	5.33	107.93	105.80
33	BA	161	A	C8-N9-C4	5.33	107.93	105.80
33	BA	307	A	N9-C4-C5	5.33	107.93	105.80
33	BA	1998	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	128	A	C8-N9-C4	5.33	107.93	105.80
1	AA	142	A	N9-C4-C5	5.33	107.93	105.80
1	AA	823	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	879	A	C4-C5-N7	-5.33	108.04	110.70
33	BA	699	A	C8-N9-C4	5.33	107.93	105.80
33	BA	1174	A	N9-C4-C5	5.33	107.93	105.80
33	BA	1490	A	N9-C4-C5	5.33	107.93	105.80
33	BA	1727	A	C4-C5-N7	-5.33	108.04	110.70
33	BA	1848	A	N9-C4-C5	5.33	107.93	105.80
1	AA	790	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	910	A	N9-C4-C5	5.33	107.93	105.80
1	AA	1297	A	C4-C5-N7	-5.33	108.04	110.70
33	BA	265	A	C4-C5-N7	-5.33	108.04	110.70
33	BA	456	A	N9-C4-C5	5.33	107.93	105.80
33	BA	475	A	N9-C4-C5	5.33	107.93	105.80
33	BA	715	A	C5-C6-N1	5.33	120.36	117.70
33	BA	2143	A	C8-N9-C4	5.33	107.93	105.80
33	BA	2462	A	N9-C4-C5	5.33	107.93	105.80
33	BA	2793	A	C4-C5-C6	5.33	119.66	117.00
33	BA	2812	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	504	A	N9-C4-C5	5.32	107.93	105.80
1	AA	679	A	N9-C4-C5	5.32	107.93	105.80
1	AA	902	A	N9-C4-C5	5.32	107.93	105.80
33	BA	44	A	C8-N9-C4	5.32	107.93	105.80
33	BA	391	A	N9-C4-C5	5.32	107.93	105.80
33	BA	762	A	N9-C4-C5	5.32	107.93	105.80
33	BA	1588	A	N9-C4-C5	5.32	107.93	105.80
33	BA	1653	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	2148	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	2505	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	2560	A	N9-C4-C5	5.32	107.93	105.80
1	AA	74	A	C8-N9-C4	5.32	107.93	105.80
1	AA	258	A	N9-C4-C5	5.32	107.93	105.80
1	AA	799	A	N9-C4-C5	5.32	107.93	105.80
33	BA	2270	A	C4-C5-N7	-5.32	108.04	110.70
34	BB	20	A	C8-N9-C4	5.32	107.93	105.80
1	AA	234	A	N9-C4-C5	5.32	107.93	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	518	A	C8-N9-C4	5.32	107.93	105.80
1	AA	724	A	N9-C4-C5	5.32	107.93	105.80
1	AA	786	A	N9-C4-C5	5.32	107.93	105.80
1	AA	899	A	N3-C4-N9	5.32	131.66	127.40
33	BA	956	A	C8-N9-C4	5.32	107.93	105.80
33	BA	1700	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	2007	A	N9-C4-C5	5.32	107.93	105.80
33	BA	2026	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	2200	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	2831	A	C8-N9-C4	5.32	107.93	105.80
1	AA	644	A	C4-C5-N7	-5.32	108.04	110.70
1	AA	1328	A	N9-C4-C5	5.32	107.93	105.80
33	BA	130	A	N9-C4-C5	5.32	107.93	105.80
21	AX	70	A	N9-C4-C5	5.32	107.93	105.80
33	BA	210	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	553	A	N9-C4-C5	5.32	107.93	105.80
33	BA	689	A	C8-N9-C4	5.32	107.93	105.80
33	BA	1074	A	N9-C4-C5	5.32	107.93	105.80
33	BA	1562	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	1956	A	C8-N9-C4	5.32	107.93	105.80
33	BA	2395	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	2455	A	N9-C4-C5	5.32	107.93	105.80
33	BA	2517	A	C4-C5-N7	-5.32	108.04	110.70
1	AA	548	A	C8-N9-C4	5.32	107.93	105.80
1	AA	617	A	C4-C5-N7	-5.32	108.04	110.70
1	AA	984	A	C4-C5-N7	-5.32	108.04	110.70
1	AA	1327	A	N9-C4-C5	5.32	107.93	105.80
1	AA	1369	A	N9-C4-C5	5.32	107.93	105.80
33	BA	84	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	230	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	486	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	727	A	N9-C4-C5	5.32	107.93	105.80
33	BA	752	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	1047	A	N9-C4-C5	5.32	107.93	105.80
33	BA	1072	A	N9-C4-C5	5.32	107.93	105.80
33	BA	1194	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	1221	A	N9-C4-C5	5.32	107.93	105.80
33	BA	1233	A	N9-C4-C5	5.32	107.93	105.80
33	BA	1302	A	N3-C4-N9	5.32	131.65	127.40
33	BA	1768	A	C8-N9-C4	5.32	107.93	105.80
33	BA	1839	A	C4-C5-N7	-5.32	108.04	110.70
33	BA	1839	A	C8-N9-C4	5.32	107.93	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	64	A	C4-C5-N7	-5.32	108.04	110.70
1	AA	161	A	C4-C5-N7	-5.31	108.04	110.70
33	BA	330	A	N9-C4-C5	5.31	107.92	105.80
33	BA	790	A	C8-N9-C4	5.31	107.93	105.80
33	BA	2616	A	C4-C5-N7	-5.31	108.04	110.70
1	AA	677	A	C4-C5-N7	-5.31	108.04	110.70
33	BA	64	A	N9-C4-C5	5.31	107.92	105.80
33	BA	337	A	N9-C4-C5	5.31	107.92	105.80
33	BA	683	A	C8-N9-C4	5.31	107.92	105.80
33	BA	1393	A	N9-C4-C5	5.31	107.92	105.80
33	BA	1919	A	C4-C5-N7	-5.31	108.04	110.70
33	BA	2066	A	C4-C5-N7	-5.31	108.04	110.70
33	BA	2662	A	C4-C5-N7	-5.31	108.04	110.70
33	BA	2794	A	N9-C4-C5	5.31	107.92	105.80
33	BA	2848	A	C4-C5-N7	-5.31	108.04	110.70
34	BB	43	A	N9-C4-C5	5.31	107.92	105.80
1	AA	107	A	N9-C4-C5	5.31	107.92	105.80
1	AA	581	A	C8-N9-C4	5.31	107.92	105.80
33	BA	490	A	N9-C4-C5	5.31	107.92	105.80
33	BA	1627	A	N9-C4-C5	5.31	107.92	105.80
33	BA	2106	A	C8-N9-C4	5.31	107.92	105.80
33	BA	2831	A	N9-C4-C5	5.31	107.92	105.80
1	AA	1014	A	N9-C4-C5	5.31	107.92	105.80
1	AA	1528	A	N9-C4-C5	5.31	107.92	105.80
33	BA	828	A	N9-C4-C5	5.31	107.92	105.80
33	BA	1027	A	N9-C4-C5	5.31	107.92	105.80
33	BA	1442	A	C5-C6-N1	5.31	120.36	117.70
33	BA	1585	A	N9-C4-C5	5.31	107.92	105.80
33	BA	1831	A	C4-C5-N7	-5.31	108.05	110.70
33	BA	2532	A	C4-C5-N7	-5.31	108.05	110.70
1	AA	711	A	C4-C5-N7	-5.31	108.05	110.70
1	AA	929	A	C8-N9-C4	5.31	107.92	105.80
33	BA	431	A	C4-C5-N7	-5.31	108.05	110.70
33	BA	1655	A	C8-N9-C4	5.31	107.92	105.80
33	BA	2454	A	C4-C5-N7	-5.31	108.05	110.70
33	BA	2547	A	N9-C4-C5	5.31	107.92	105.80
1	AA	150	A	C4-C5-C6	5.31	119.65	117.00
1	AA	308	A	C8-N9-C4	5.31	107.92	105.80
1	AA	705	A	N9-C4-C5	5.31	107.92	105.80
33	BA	715	A	C4-C5-N7	-5.31	108.05	110.70
33	BA	830	A	C4-C5-N7	-5.31	108.05	110.70
33	BA	1244	A	C8-N9-C4	5.31	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1340	A	C8-N9-C4	5.31	107.92	105.80
33	BA	1816	A	C5-C6-N1	5.31	120.35	117.70
33	BA	2343	A	N9-C4-C5	5.31	107.92	105.80
33	BA	2691	A	C8-N9-C4	5.31	107.92	105.80
33	BA	2900	A	N9-C4-C5	5.31	107.92	105.80
1	AA	81	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	52	A	N9-C4-C5	5.30	107.92	105.80
33	BA	339	A	N9-C4-C5	5.30	107.92	105.80
33	BA	634	A	N9-C4-C5	5.30	107.92	105.80
33	BA	705	A	N9-C4-C5	5.30	107.92	105.80
33	BA	943	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	1675	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	1802	A	N9-C4-C5	5.30	107.92	105.80
33	BA	2830	A	N9-C4-C5	5.30	107.92	105.80
33	BA	2923	A	N9-C4-C5	5.30	107.92	105.80
1	AA	978	A	C8-N9-C4	5.30	107.92	105.80
1	AA	1278	A	N9-C4-C5	5.30	107.92	105.80
33	BA	260	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	2340	A	N9-C4-C5	5.30	107.92	105.80
1	AA	457	A	C4-C5-C6	5.30	119.65	117.00
1	AA	671	A	N9-C4-C5	5.30	107.92	105.80
1	AA	743	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	236	A	N9-C4-C5	5.30	107.92	105.80
33	BA	870	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	1034	A	N9-C4-C5	5.30	107.92	105.80
33	BA	1054	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	1412	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	1461	A	N9-C4-C5	5.30	107.92	105.80
33	BA	1575	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	1925	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	2794	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	674	A	C4-C5-C6	5.30	119.65	117.00
1	AA	1206	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	28	A	N9-C4-C5	5.30	107.92	105.80
33	BA	150	A	N9-C4-C5	5.30	107.92	105.80
33	BA	391	A	C8-N9-C4	5.30	107.92	105.80
33	BA	421	A	N9-C4-C5	5.30	107.92	105.80
33	BA	763	A	N9-C4-C5	5.30	107.92	105.80
33	BA	1014	A	N9-C4-C5	5.30	107.92	105.80
33	BA	1179	A	N9-C4-C5	5.30	107.92	105.80
33	BA	1638	A	C5-C6-N1	5.30	120.35	117.70
33	BA	1905	A	C8-N9-C4	5.30	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2390	A	N9-C4-C5	5.30	107.92	105.80
33	BA	2421	A	N9-C4-C5	5.30	107.92	105.80
1	AA	674	A	C8-N9-C4	5.30	107.92	105.80
33	BA	118	A	C4-C5-C6	5.30	119.65	117.00
33	BA	194	A	N9-C4-C5	5.30	107.92	105.80
33	BA	958	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	2032	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	2505	A	N9-C4-C5	5.30	107.92	105.80
33	BA	2826	A	C8-N9-C4	5.30	107.92	105.80
1	AA	913	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	985	A	N9-C4-C5	5.30	107.92	105.80
33	BA	524	A	N9-C4-C5	5.30	107.92	105.80
33	BA	1149	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	1485	A	N9-C4-C5	5.30	107.92	105.80
33	BA	1672	A	C4-C5-N7	-5.30	108.05	110.70
33	BA	1710	A	C5-C6-N1	5.30	120.35	117.70
33	BA	2831	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	1493	A	N9-C4-C5	5.29	107.92	105.80
33	BA	2252	A	N9-C4-C5	5.29	107.92	105.80
1	AA	616	A	N9-C4-C5	5.29	107.92	105.80
1	AA	1451	A	N9-C4-C5	5.29	107.92	105.80
1	AA	1470	A	C4-C5-N7	-5.29	108.05	110.70
22	AY	2	G	C4'-C3'-C2'	-5.29	97.31	102.60
33	BA	226	A	C5-C6-N1	5.29	120.35	117.70
33	BA	560	A	C4-C5-N7	-5.29	108.05	110.70
33	BA	659	A	C4-C5-N7	-5.29	108.05	110.70
33	BA	1919	A	N3-C4-N9	5.29	131.63	127.40
1	AA	975	A	C4-C5-N7	-5.29	108.05	110.70
1	AA	1341	A	N9-C4-C5	5.29	107.92	105.80
33	BA	623	A	N9-C4-C5	5.29	107.92	105.80
33	BA	790	A	N9-C4-C5	5.29	107.92	105.80
33	BA	1005	A	C8-N9-C4	5.29	107.92	105.80
33	BA	1517	A	N9-C4-C5	5.29	107.92	105.80
33	BA	2296	A	C4-C5-N7	-5.29	108.05	110.70
33	BA	2329	A	C5-C6-N1	5.29	120.34	117.70
1	AA	460	A	N9-C4-C5	5.29	107.92	105.80
33	BA	630	A	C4-C5-N7	-5.29	108.06	110.70
33	BA	1947	A	N9-C4-C5	5.29	107.92	105.80
1	AA	211	A	N9-C4-C5	5.29	107.92	105.80
1	AA	650	A	C4-C5-N7	-5.29	108.06	110.70
1	AA	672	A	N9-C4-C5	5.29	107.92	105.80
33	BA	388	A	N9-C4-C5	5.29	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	882	A	C4-C5-N7	-5.29	108.06	110.70
33	BA	1335	A	N9-C4-C5	5.29	107.92	105.80
33	BA	1375	A	N9-C4-C5	5.29	107.92	105.80
33	BA	1832	A	C8-N9-C4	5.29	107.92	105.80
33	BA	1888	A	C4-C5-N7	-5.29	108.06	110.70
33	BA	1895	A	N9-C4-C5	5.29	107.92	105.80
1	AA	730	A	C4-C5-N7	-5.29	108.06	110.70
21	AX	76	A	C4-C5-N7	-5.29	108.06	110.70
33	BA	1618	A	C8-N9-C4	5.29	107.92	105.80
1	AA	81	A	N9-C4-C5	5.29	107.91	105.80
1	AA	117	A	C4-C5-N7	-5.29	108.06	110.70
33	BA	889	A	N9-C4-C5	5.29	107.91	105.80
33	BA	952	A	N9-C4-C5	5.29	107.91	105.80
33	BA	1286	A	N9-C4-C5	5.29	107.91	105.80
33	BA	1417	A	N3-C4-N9	5.29	131.63	127.40
33	BA	1648	A	C4-C5-N7	-5.29	108.06	110.70
33	BA	2027	A	C4-C5-N7	-5.29	108.06	110.70
33	BA	2059	A	C4-C5-N7	-5.29	108.06	110.70
1	AA	35	A	N9-C4-C5	5.28	107.91	105.80
1	AA	1456	A	N9-C4-C5	5.28	107.91	105.80
33	BA	247	A	C8-N9-C4	5.28	107.91	105.80
33	BA	866	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	1432	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	1900	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	2252	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	2844	A	C8-N9-C4	5.28	107.91	105.80
33	BA	2851	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	808	A	N9-C4-C5	5.28	107.91	105.80
33	BA	1813	A	N9-C4-C5	5.28	107.91	105.80
33	BA	2619	A	N9-C4-C5	5.28	107.91	105.80
1	AA	301	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	1405	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	1513	A	N9-C4-C5	5.28	107.91	105.80
33	BA	6	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	647	A	N9-C4-C5	5.28	107.91	105.80
33	BA	692	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	948	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	1778	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	1913	A	N9-C4-C5	5.28	107.91	105.80
33	BA	2719	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	390	A	C8-N9-C4	5.28	107.91	105.80
1	AA	917	A	N9-C4-C5	5.28	107.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	437	A	C8-N9-C4	5.28	107.91	105.80
33	BA	549	A	N9-C4-C5	5.28	107.91	105.80
33	BA	1680	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	2402	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	2919	A	N9-C4-C5	5.28	107.91	105.80
1	AA	1261	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	526	A	C5-C6-N1	5.28	120.34	117.70
33	BA	2123	A	C8-N9-C4	5.28	107.91	105.80
1	AA	724	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	1392	A	N9-C4-C5	5.28	107.91	105.80
33	BA	1404	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	1709	A	C4-C5-N7	-5.28	108.06	110.70
33	BA	1722	A	N9-C4-C5	5.28	107.91	105.80
33	BA	2032	A	N9-C4-C5	5.28	107.91	105.80
21	AX	76	A	N9-C4-C5	5.27	107.91	105.80
33	BA	1685	A	N9-C4-C5	5.27	107.91	105.80
33	BA	2044	A	N9-C4-C5	5.27	107.91	105.80
1	AA	568	A	N9-C4-C5	5.27	107.91	105.80
1	AA	823	A	N9-C4-C5	5.27	107.91	105.80
33	BA	318	A	N9-C4-C5	5.27	107.91	105.80
33	BA	559	A	C4-C5-N7	-5.27	108.06	110.70
33	BA	656	A	C8-N9-C4	5.27	107.91	105.80
33	BA	993	A	C4-C5-N7	-5.27	108.06	110.70
33	BA	1291	A	C4-C5-N7	-5.27	108.06	110.70
33	BA	1562	A	N9-C4-C5	5.27	107.91	105.80
33	BA	2052	A	N9-C4-C5	5.27	107.91	105.80
33	BA	2339	A	C8-N9-C4	5.27	107.91	105.80
1	AA	61	A	N9-C4-C5	5.27	107.91	105.80
33	BA	1357	A	N9-C4-C5	5.27	107.91	105.80
1	AA	72	A	N9-C4-C5	5.27	107.91	105.80
33	BA	1131	A	C4-C5-N7	-5.27	108.06	110.70
33	BA	1417	A	C4-C5-C6	5.27	119.64	117.00
33	BA	1614	A	N9-C4-C5	5.27	107.91	105.80
33	BA	1615	A	C4-C5-N7	-5.27	108.06	110.70
33	BA	1999	A	C4-C5-N7	-5.27	108.06	110.70
33	BA	2500	A	N9-C4-C5	5.27	107.91	105.80
1	AA	76	A	C4-C5-N7	-5.27	108.07	110.70
1	AA	361	A	C4-C5-N7	-5.27	108.07	110.70
33	BA	53	A	C8-N9-C4	5.27	107.91	105.80
33	BA	391	A	C4-C5-N7	-5.27	108.07	110.70
33	BA	1008	A	N9-C4-C5	5.27	107.91	105.80
33	BA	1480	A	C8-N9-C4	5.27	107.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1536	A	C4-C5-N7	-5.27	108.07	110.70
33	BA	2044	A	C4-C5-N7	-5.27	108.07	110.70
33	BA	2059	A	N9-C4-C5	5.27	107.91	105.80
33	BA	2459	A	C4-C5-N7	-5.27	108.07	110.70
33	BA	774	A	C5-C6-N1	5.27	120.33	117.70
33	BA	948	A	C8-N9-C4	5.27	107.91	105.80
1	AA	382	A	N9-C4-C5	5.26	107.91	105.80
21	AX	9	A	C4-C5-N7	-5.26	108.07	110.70
33	BA	108	A	C4-C5-N7	-5.26	108.07	110.70
33	BA	390	A	N9-C4-C5	5.26	107.91	105.80
33	BA	623	A	C4-C5-N7	-5.26	108.07	110.70
33	BA	1244	A	C4-C5-N7	-5.26	108.07	110.70
33	BA	1480	A	C4-C5-N7	-5.26	108.07	110.70
33	BA	1583	A	N9-C4-C5	5.26	107.91	105.80
33	BA	1961	A	N9-C4-C5	5.26	107.91	105.80
1	AA	684	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	743	A	N9-C4-C5	5.26	107.91	105.80
33	BA	1655	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	128	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	433	A	N9-C4-C5	5.26	107.91	105.80
1	AA	758	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	1355	A	N3-C4-N9	5.26	131.61	127.40
33	BA	133	A	C4-C5-N7	-5.26	108.07	110.70
33	BA	494	A	C8-N9-C4	5.26	107.91	105.80
33	BA	1426	A	N9-C4-C5	5.26	107.90	105.80
33	BA	1434	A	C8-N9-C4	5.26	107.91	105.80
33	BA	2124	A	C4-C5-N7	-5.26	108.07	110.70
33	BA	2369	A	N9-C4-C5	5.26	107.91	105.80
34	BB	25	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	1296	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	1407	A	N9-C4-C5	5.26	107.90	105.80
33	BA	38	A	C8-N9-C4	5.26	107.90	105.80
33	BA	179	A	C8-N9-C4	5.26	107.90	105.80
33	BA	2402	A	N9-C4-C5	5.26	107.90	105.80
33	BA	943	A	N9-C4-C5	5.26	107.90	105.80
33	BA	1253	A	C4-C5-N7	-5.26	108.07	110.70
33	BA	2026	A	C5-C6-N1	5.26	120.33	117.70
33	BA	2117	A	C5-C6-N1	5.26	120.33	117.70
33	BA	2402	A	C5-C6-N1	5.26	120.33	117.70
33	BA	2750	A	N9-C4-C5	5.26	107.90	105.80
1	AA	18	A	N9-C4-C5	5.26	107.90	105.80
1	AA	1155	A	C4-C5-N7	-5.26	108.07	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1206	A	N9-C4-C5	5.26	107.90	105.80
1	AA	1384	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	1463	A	C4-C5-N7	-5.26	108.07	110.70
33	BA	305	A	C4-C5-N7	-5.26	108.07	110.70
33	BA	459	A	N9-C4-C5	5.26	107.90	105.80
33	BA	835	A	N9-C4-C5	5.26	107.90	105.80
33	BA	2316	A	N9-C4-C5	5.26	107.90	105.80
1	AA	604	A	N9-C4-C5	5.25	107.90	105.80
1	AA	911	A	C8-N9-C4	5.25	107.90	105.80
33	BA	1490	A	C5-C6-N1	5.25	120.33	117.70
33	BA	2887	A	C4-C5-N7	-5.25	108.07	110.70
1	AA	1112	A	N9-C4-C5	5.25	107.90	105.80
21	AX	24	A	C5-C6-N1	5.25	120.33	117.70
33	BA	21	A	C4-C5-N7	-5.25	108.07	110.70
33	BA	84	A	N9-C4-C5	5.25	107.90	105.80
33	BA	193	A	N9-C4-C5	5.25	107.90	105.80
33	BA	1294	A	C4'-C3'-O3'	-5.25	98.37	109.40
33	BA	1614	A	C8-N9-C4	5.25	107.90	105.80
33	BA	2844	A	C4-C5-N7	-5.25	108.07	110.70
1	AA	1383	A	N9-C4-C5	5.25	107.90	105.80
1	AA	1490	A	N9-C4-C5	5.25	107.90	105.80
33	BA	13	A	N9-C4-C5	5.25	107.90	105.80
33	BA	254	A	N9-C4-C5	5.25	107.90	105.80
33	BA	1340	A	C4-C5-N7	-5.25	108.07	110.70
33	BA	1768	A	C4-C5-N7	-5.25	108.07	110.70
33	BA	2595	A	C8-N9-C4	5.25	107.90	105.80
33	BA	2754	A	N9-C4-C5	5.25	107.90	105.80
34	BB	20	A	N9-C4-C5	5.25	107.90	105.80
1	AA	344	A	C4-C5-N7	-5.25	108.08	110.70
33	BA	2228	A	C4-C5-N7	-5.25	108.08	110.70
1	AA	140	A	N9-C4-C5	5.25	107.90	105.80
1	AA	364	A	C5-C6-N1	5.25	120.33	117.70
1	AA	477	A	C8-N9-C4	5.25	107.90	105.80
1	AA	1247	A	N3-C4-N9	5.25	131.60	127.40
33	BA	530	A	N9-C4-C5	5.25	107.90	105.80
33	BA	1149	A	N9-C4-C5	5.25	107.90	105.80
33	BA	1900	A	C8-N9-C4	5.25	107.90	105.80
33	BA	2339	A	C4-C5-N7	-5.25	108.08	110.70
33	BA	659	A	N9-C4-C5	5.25	107.90	105.80
33	BA	1075	A	N9-C4-C5	5.25	107.90	105.80
33	BA	1258	A	C4-C5-N7	-5.25	108.08	110.70
33	BA	1286	A	C5-C6-N1	5.25	120.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1316	A	C4-C5-N7	-5.25	108.08	110.70
33	BA	2754	A	C5-C6-N1	5.25	120.32	117.70
34	BB	46	A	C5-C6-N1	5.25	120.32	117.70
1	AA	605	A	C4-C5-N7	-5.25	108.08	110.70
33	BA	634	A	C5-C6-N1	5.25	120.32	117.70
33	BA	1655	A	N9-C4-C5	5.25	107.90	105.80
33	BA	185	A	N9-C4-C5	5.24	107.90	105.80
33	BA	616	A	C4-C5-N7	-5.24	108.08	110.70
33	BA	1721	A	N9-C4-C5	5.24	107.90	105.80
1	AA	346	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	1004	A	N9-C4-C5	5.24	107.90	105.80
33	BA	537	A	C4-C5-N7	-5.24	108.08	110.70
33	BA	1520	A	C5-C6-N1	5.24	120.32	117.70
1	AA	1463	A	N9-C4-C5	5.24	107.90	105.80
33	BA	216	A	N9-C4-C5	5.24	107.90	105.80
33	BA	538	A	C4-C5-N7	-5.24	108.08	110.70
33	BA	1188	A	C8-N9-C4	5.24	107.90	105.80
33	BA	1197	A	C4-C5-N7	-5.24	108.08	110.70
33	BA	1555	A	N3-C4-N9	5.24	131.59	127.40
33	BA	2252	A	C8-N9-C4	5.24	107.90	105.80
33	BA	2532	A	N9-C4-C5	5.24	107.90	105.80
33	BA	2916	A	C8-N9-C4	5.24	107.90	105.80
1	AA	1160	A	C5-C6-N1	5.24	120.32	117.70
1	AA	1247	A	C4-C5-C6	5.24	119.62	117.00
33	BA	61	A	C4-C5-N7	-5.24	108.08	110.70
33	BA	95	A	C5-C6-N1	5.24	120.32	117.70
33	BA	964	A	C4-C5-N7	-5.24	108.08	110.70
33	BA	1054	A	N9-C4-C5	5.24	107.89	105.80
33	BA	1876	A	C8-N9-C4	5.24	107.89	105.80
33	BA	2205	A	C4-C5-N7	-5.24	108.08	110.70
33	BA	2893	A	N9-C4-C5	5.24	107.89	105.80
33	BA	1618	A	C4-C5-N7	-5.24	108.08	110.70
33	BA	2164	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	730	A	N9-C4-C5	5.24	107.89	105.80
1	AA	1128	A	C8-N9-C4	5.24	107.89	105.80
33	BA	1103	A	C5-C6-N1	5.24	120.32	117.70
33	BA	1188	A	N3-C4-N9	5.24	131.59	127.40
33	BA	2349	A	C4-C5-N7	-5.24	108.08	110.70
33	BA	2498	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	984	A	N9-C4-C5	5.23	107.89	105.80
1	AA	1315	A	C8-N9-C4	5.23	107.89	105.80
33	BA	593	A	C5-C6-N1	5.23	120.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1477	A	C4-C5-N7	-5.23	108.08	110.70
33	BA	2889	A	N9-C4-C5	5.23	107.89	105.80
1	AA	605	A	C5-C6-N1	5.23	120.32	117.70
1	AA	713	A	C4-C5-N7	-5.23	108.08	110.70
33	BA	690	A	N9-C4-C5	5.23	107.89	105.80
1	AA	933	A	C5-C6-N1	5.23	120.32	117.70
33	BA	1100	A	C4-C5-N7	-5.23	108.08	110.70
33	BA	1126	A	C4-C5-N7	-5.23	108.08	110.70
33	BA	2754	A	C4-C5-N7	-5.23	108.08	110.70
33	BA	2846	A	N9-C4-C5	5.23	107.89	105.80
1	AA	335	A	C4-C5-N7	-5.23	108.09	110.70
33	BA	1360	A	C4-C5-N7	-5.23	108.08	110.70
33	BA	2270	A	N9-C4-C5	5.23	107.89	105.80
1	AA	57	A	N9-C4-C5	5.23	107.89	105.80
1	AA	1167	C	C6-N1-C1'	-5.23	114.53	120.80
1	AA	1270	A	N9-C4-C5	5.23	107.89	105.80
33	BA	647	A	C4-C5-C6	5.23	119.61	117.00
33	BA	947	A	N9-C4-C5	5.23	107.89	105.80
33	BA	1524	A	N9-C4-C5	5.23	107.89	105.80
33	BA	2066	A	N9-C4-C5	5.23	107.89	105.80
33	BA	2106	A	N9-C4-C5	5.23	107.89	105.80
33	BA	2358	A	C5-C6-N1	5.23	120.31	117.70
33	BA	2381	A	C4-C5-N7	-5.23	108.09	110.70
33	BA	2532	A	C8-N9-C4	5.23	107.89	105.80
1	AA	844	A	C4-C5-N7	-5.23	108.09	110.70
33	BA	275	A	C8-N9-C4	5.23	107.89	105.80
33	BA	1614	A	C4-C5-N7	-5.23	108.09	110.70
33	BA	1814	A	N3-C4-N9	5.23	131.58	127.40
33	BA	2708	A	N9-C4-C5	5.23	107.89	105.80
33	BA	2787	A	N9-C4-C5	5.23	107.89	105.80
33	BA	2810	A	N9-C4-C5	5.23	107.89	105.80
1	AA	512	A	N9-C4-C5	5.22	107.89	105.80
1	AA	611	A	N9-C4-C5	5.22	107.89	105.80
1	AA	758	A	C5-C6-N1	5.22	120.31	117.70
1	AA	844	A	C5-C6-N1	5.22	120.31	117.70
1	AA	1176	A	N9-C4-C5	5.22	107.89	105.80
22	AY	2	G	C4'-C3'-O3'	5.22	123.45	113.00
33	BA	171	A	C4-C5-N7	-5.22	108.09	110.70
33	BA	970	A	C4-C5-N7	-5.22	108.09	110.70
33	BA	1134	A	C5-C6-N1	5.22	120.31	117.70
33	BA	1222	A	C4-C5-N7	-5.22	108.09	110.70
33	BA	2407	A	C8-N9-C4	5.22	107.89	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2790	A	C5-C6-N1	5.22	120.31	117.70
34	BB	64	A	N9-C4-C5	5.22	107.89	105.80
1	AA	1016	A	C8-N9-C4	5.22	107.89	105.80
1	AA	1234	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	1366	A	N9-C4-C5	5.22	107.89	105.80
1	AA	1478	A	C4-C5-N7	-5.22	108.09	110.70
33	BA	118	A	C5-C6-N1	5.22	120.31	117.70
33	BA	156	A	C4-C5-N7	-5.22	108.09	110.70
33	BA	1284	A	C4-C5-N7	-5.22	108.09	110.70
33	BA	2735	A	C5-C6-N1	5.22	120.31	117.70
1	AA	94	A	N9-C4-C5	5.22	107.89	105.80
1	AA	644	A	N9-C4-C5	5.22	107.89	105.80
1	AA	684	A	N9-C4-C5	5.22	107.89	105.80
33	BA	2436	A	C5-C6-N1	5.22	120.31	117.70
1	AA	118	A	N9-C4-C5	5.22	107.89	105.80
1	AA	151	A	C4-C5-C6	5.22	119.61	117.00
33	BA	230	A	N9-C4-C5	5.22	107.89	105.80
33	BA	1308	A	N9-C4-C5	5.22	107.89	105.80
33	BA	1473	A	C4-C5-C6	5.22	119.61	117.00
33	BA	1721	A	C4-C5-N7	-5.22	108.09	110.70
33	BA	1967	A	N9-C4-C5	5.22	107.89	105.80
33	BA	2303	A	C8-N9-C4	5.22	107.89	105.80
33	BA	2468	A	N9-C4-C5	5.22	107.89	105.80
33	BA	260	A	N9-C4-C5	5.22	107.89	105.80
33	BA	1667	A	C8-N9-C4	5.22	107.89	105.80
33	BA	2844	A	C5-C6-N1	5.22	120.31	117.70
1	AA	975	A	N9-C4-C5	5.22	107.89	105.80
1	AA	1022	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	1143	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	1294	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	1348	A	N9-C4-C5	5.22	107.89	105.80
33	BA	1197	A	N9-C4-C5	5.22	107.89	105.80
33	BA	2241	A	C8-N9-C4	5.22	107.89	105.80
33	BA	2349	A	N9-C4-C5	5.22	107.89	105.80
1	AA	278	A	C4-C5-N7	-5.21	108.09	110.70
1	AA	381	A	C4-C5-N7	-5.21	108.09	110.70
1	AA	649	A	C4-C5-N7	-5.21	108.09	110.70
1	AA	899	A	C4-C5-C6	5.21	119.61	117.00
1	AA	1188	A	C4-C5-N7	-5.21	108.09	110.70
33	BA	1042	A	C4-C5-N7	-5.21	108.09	110.70
33	BA	2441	A	C4-C5-N7	-5.21	108.09	110.70
33	BA	2790	A	C4-C5-N7	-5.21	108.09	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2827	A	N9-C4-C5	5.21	107.89	105.80
33	BA	753	A	N9-C4-C5	5.21	107.89	105.80
33	BA	2860	A	N9-C4-C5	5.21	107.89	105.80
1	AA	129	A	N9-C4-C5	5.21	107.88	105.80
1	AA	337	A	C4-C5-N7	-5.21	108.09	110.70
33	BA	619	A	N9-C4-C5	5.21	107.89	105.80
33	BA	667	A	C8-N9-C4	5.21	107.89	105.80
33	BA	971	A	N9-C4-C5	5.21	107.88	105.80
33	BA	1190	A	N9-C4-C5	5.21	107.88	105.80
33	BA	2044	A	C8-N9-C4	5.21	107.89	105.80
33	BA	496	A	C5-C6-N1	5.21	120.31	117.70
33	BA	1491	A	N9-C4-C5	5.21	107.88	105.80
33	BA	1776	A	C4-C5-N7	-5.21	108.09	110.70
33	BA	1778	A	C8-N9-C4	5.21	107.88	105.80
1	AA	630	A	C8-N9-C4	5.21	107.88	105.80
1	AA	1245	A	C4-C5-N7	-5.21	108.10	110.70
33	BA	41	A	C4-C5-N7	-5.21	108.10	110.70
33	BA	494	A	C4-C5-N7	-5.21	108.09	110.70
33	BA	622	A	C8-N9-C4	5.21	107.88	105.80
33	BA	630	A	N9-C4-C5	5.21	107.88	105.80
33	BA	1536	A	C8-N9-C4	5.21	107.88	105.80
33	BA	2163	A	C4-C5-N7	-5.21	108.09	110.70
33	BA	2329	A	N9-C4-C5	5.21	107.88	105.80
1	AA	758	A	N9-C4-C5	5.21	107.88	105.80
1	AA	1022	A	N9-C4-C5	5.21	107.88	105.80
33	BA	254	A	C4-C5-N7	-5.21	108.10	110.70
33	BA	574	A	C8-N9-C4	5.21	107.88	105.80
33	BA	1265	A	C8-N9-C4	5.21	107.88	105.80
33	BA	2663	A	C4-C5-N7	-5.21	108.10	110.70
34	BB	11	A	C8-N9-C4	5.21	107.88	105.80
1	AA	838	A	C5-C6-N1	5.21	120.30	117.70
33	BA	1845	A	N9-C4-C5	5.21	107.88	105.80
33	BA	53	A	C4-C5-N7	-5.20	108.10	110.70
33	BA	258	A	C4-C5-N7	-5.20	108.10	110.70
33	BA	560	A	C5-C6-N1	5.20	120.30	117.70
33	BA	2468	A	C8-N9-C4	5.20	107.88	105.80
33	BA	2812	A	C5-C6-N1	5.20	120.30	117.70
1	AA	659	A	N9-C4-C5	5.20	107.88	105.80
1	AA	1315	A	N9-C4-C5	5.20	107.88	105.80
33	BA	71	A	N9-C4-C5	5.20	107.88	105.80
33	BA	2734	A	N9-C4-C5	5.20	107.88	105.80
34	BB	46	A	C4-C5-N7	-5.20	108.10	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	6	A	N9-C4-C5	5.20	107.88	105.80
33	BA	486	A	N9-C4-C5	5.20	107.88	105.80
33	BA	868	A	N9-C4-C5	5.20	107.88	105.80
1	AA	631	A	N3-C4-N9	5.20	131.56	127.40
1	AA	838	A	C4-C5-N7	-5.20	108.10	110.70
1	AA	1189	A	C8-N9-C4	5.20	107.88	105.80
33	BA	537	A	N9-C4-C5	5.20	107.88	105.80
33	BA	993	A	N9-C4-C5	5.20	107.88	105.80
33	BA	1485	A	C4-C5-N7	-5.20	108.10	110.70
33	BA	1774	A	C8-N9-C4	5.20	107.88	105.80
1	AA	1179	A	N9-C4-C5	5.20	107.88	105.80
33	BA	724	A	C4-C5-N7	-5.20	108.10	110.70
33	BA	1680	A	N9-C4-C5	5.20	107.88	105.80
1	AA	344	A	N9-C4-C5	5.20	107.88	105.80
1	AA	532	A	N9-C4-C5	5.20	107.88	105.80
1	AA	1133	A	N3-C4-N9	5.20	131.56	127.40
33	BA	925	A	C8-N9-C4	5.20	107.88	105.80
33	BA	1608	A	N9-C4-C5	5.20	107.88	105.80
33	BA	1727	A	N9-C4-C5	5.20	107.88	105.80
33	BA	2027	A	N9-C4-C5	5.20	107.88	105.80
33	BA	2062	A	N3-C4-N9	5.20	131.56	127.40
33	BA	2083	A	C4-C5-N7	-5.20	108.10	110.70
33	BA	2459	A	C8-N9-C4	5.20	107.88	105.80
1	AA	439	A	C4-C5-N7	-5.19	108.10	110.70
1	AA	844	A	N9-C4-C5	5.19	107.88	105.80
33	BA	841	A	C4-C5-N7	-5.19	108.10	110.70
1	AA	507	A	C5-C6-N6	-5.19	119.55	123.70
1	AA	913	A	N9-C4-C5	5.19	107.88	105.80
1	AA	993	A	N9-C4-C5	5.19	107.88	105.80
33	BA	518	A	N9-C4-C5	5.19	107.88	105.80
33	BA	1619	A	N9-C4-C5	5.19	107.88	105.80
33	BA	1778	A	N9-C4-C5	5.19	107.88	105.80
33	BA	2358	A	N9-C4-C5	5.19	107.88	105.80
1	AA	114	A	C4-C5-N7	-5.19	108.11	110.70
1	AA	462	A	N9-C4-C5	5.19	107.88	105.80
33	BA	971	A	C4-C5-N7	-5.19	108.10	110.70
33	BA	2770	A	N9-C4-C5	5.19	107.88	105.80
33	BA	2862	A	C5-C6-N1	5.19	120.30	117.70
1	AA	1167	C	N3-C2-O2	-5.19	118.27	121.90
33	BA	790	A	C4-C5-N7	-5.19	108.11	110.70
33	BA	1075	A	C8-N9-C4	5.19	107.88	105.80
33	BA	2124	A	N9-C4-C5	5.19	107.88	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2164	A	C8-N9-C4	5.19	107.88	105.80
33	BA	551	A	N9-C4-C5	5.19	107.87	105.80
33	BA	1575	A	N9-C4-C5	5.19	107.87	105.80
1	AA	120	A	N9-C4-C5	5.18	107.87	105.80
1	AA	933	A	N9-C4-C5	5.18	107.87	105.80
33	BA	616	A	N9-C4-C5	5.18	107.87	105.80
33	BA	1491	A	C4-C5-N7	-5.18	108.11	110.70
33	BA	2080	A	C4-C5-N7	-5.18	108.11	110.70
33	BA	2349	A	C8-N9-C4	5.18	107.87	105.80
1	AA	617	A	N9-C4-C5	5.18	107.87	105.80
33	BA	108	A	C5-C6-N1	5.18	120.29	117.70
33	BA	2498	A	N9-C4-C5	5.18	107.87	105.80
33	BA	2662	A	N9-C4-C5	5.18	107.87	105.80
33	BA	504	A	C4-C5-C6	5.18	119.59	117.00
33	BA	183	A	C4-C5-C6	5.18	119.59	117.00
33	BA	504	A	C5-C6-N1	5.18	120.29	117.70
33	BA	1778	A	C5-C6-N1	5.18	120.29	117.70
1	AA	1133	A	C8-N9-C4	5.18	107.87	105.80
33	BA	1258	A	C5-C6-N1	5.18	120.29	117.70
33	BA	1536	A	N9-C4-C5	5.18	107.87	105.80
33	BA	2302	A	N9-C4-C5	5.18	107.87	105.80
1	AA	381	A	N9-C4-C5	5.18	107.87	105.80
1	AA	879	A	N9-C4-C5	5.18	107.87	105.80
1	AA	1297	A	N9-C4-C5	5.18	107.87	105.80
33	BA	1919	A	C8-N9-C4	5.18	107.87	105.80
33	BA	2339	A	N9-C4-C5	5.18	107.87	105.80
1	AA	161	A	N9-C4-C5	5.17	107.87	105.80
1	AA	282	A	C5-C6-N1	5.17	120.29	117.70
1	AA	874	A	C4-C5-N7	-5.17	108.11	110.70
1	AA	1272	A	C5-C6-N1	5.17	120.29	117.70
33	BA	1291	A	N9-C4-C5	5.17	107.87	105.80
33	BA	1768	A	N9-C4-C5	5.17	107.87	105.80
33	BA	1814	A	C4-C5-C6	5.17	119.59	117.00
33	BA	1900	A	N9-C4-C5	5.17	107.87	105.80
1	AA	1161	A	N9-C4-C5	5.17	107.87	105.80
33	BA	21	A	N9-C4-C5	5.17	107.87	105.80
33	BA	168	A	C4-C5-N7	-5.17	108.11	110.70
33	BA	1581	A	N9-C4-C5	5.17	107.87	105.80
1	AA	117	A	N9-C4-C5	5.17	107.87	105.80
1	AA	725	A	C8-N9-C4	5.17	107.87	105.80
33	BA	689	A	C4-C5-N7	-5.17	108.11	110.70
33	BA	1046	A	C5-C6-N1	5.17	120.29	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2228	A	N9-C4-C5	5.17	107.87	105.80
33	BA	658	A	C8-N9-C4	5.17	107.87	105.80
33	BA	948	A	N9-C4-C5	5.17	107.87	105.80
33	BA	324	A	N9-C4-C5	5.17	107.87	105.80
33	BA	1695	A	C4-C5-N7	-5.17	108.12	110.70
33	BA	647	A	C4-C5-N7	-5.17	108.12	110.70
33	BA	2887	A	N9-C4-C5	5.17	107.87	105.80
1	AA	1284	A	N9-C4-C5	5.16	107.86	105.80
33	BA	431	A	N9-C4-C5	5.16	107.86	105.80
33	BA	970	A	C5-C6-N1	5.16	120.28	117.70
33	BA	1901	A	C4-C5-N7	-5.16	108.12	110.70
33	BA	486	A	C5-C6-N1	5.16	120.28	117.70
33	BA	913	A	C5-C6-N1	5.16	120.28	117.70
33	BA	1360	A	N9-C4-C5	5.16	107.86	105.80
1	AA	308	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	519	A	C8-N9-C4	5.16	107.86	105.80
33	BA	560	A	C8-N9-C4	5.16	107.86	105.80
33	BA	956	A	C4-C5-N7	-5.16	108.12	110.70
33	BA	2689	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	711	A	N9-C4-C5	5.16	107.86	105.80
1	AA	1272	A	C4-C5-N7	-5.16	108.12	110.70
33	BA	1201	A	N3-C4-N9	5.16	131.53	127.40
33	BA	1360	A	C8-N9-C4	5.16	107.86	105.80
33	BA	1945	A	C8-N9-C4	5.16	107.86	105.80
33	BA	2164	A	N9-C4-C5	5.16	107.86	105.80
1	AA	1197	A	N9-C4-C5	5.16	107.86	105.80
33	BA	1073	A	N9-C4-C5	5.16	107.86	105.80
33	BA	2689	A	N9-C4-C5	5.16	107.86	105.80
1	AA	677	A	N9-C4-C5	5.16	107.86	105.80
1	AA	1016	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	1161	A	C4-C5-N7	-5.16	108.12	110.70
33	BA	1581	A	C5-C6-N1	5.16	120.28	117.70
33	BA	1653	A	N9-C4-C5	5.16	107.86	105.80
33	BA	2205	A	N9-C4-C5	5.16	107.86	105.80
33	BA	2441	A	N9-C4-C5	5.16	107.86	105.80
33	BA	2898	A	C4-C5-C6	5.15	119.58	117.00
1	AA	918	A	N9-C4-C5	5.15	107.86	105.80
33	BA	133	A	N9-C4-C5	5.15	107.86	105.80
33	BA	369	A	N9-C4-C5	5.15	107.86	105.80
33	BA	1404	A	N9-C4-C5	5.15	107.86	105.80
33	BA	1672	A	C5-C6-N1	5.15	120.28	117.70
33	BA	2616	A	C8-N9-C4	5.15	107.86	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2719	A	N9-C4-C5	5.15	107.86	105.80
1	AA	1288	A	C4-C5-N7	-5.15	108.12	110.70
1	AA	1405	A	N9-C4-C5	5.15	107.86	105.80
33	BA	956	A	N9-C4-C5	5.15	107.86	105.80
33	BA	1096	A	C8-N9-C4	5.15	107.86	105.80
33	BA	1305	A	N3-C4-N9	5.15	131.52	127.40
33	BA	1638	A	C4-C5-N7	-5.15	108.12	110.70
1	AA	114	A	C8-N9-C4	5.15	107.86	105.80
1	AA	572	A	C4-C5-N7	-5.15	108.12	110.70
1	AA	875	A	C5-C6-N1	5.15	120.27	117.70
1	AA	911	A	C4-C5-N7	-5.15	108.12	110.70
33	BA	1581	A	C4-C5-N7	-5.15	108.13	110.70
33	BA	2463	A	C8-N9-C4	5.15	107.86	105.80
33	BA	117	A	C8-N9-C4	5.15	107.86	105.80
33	BA	1046	A	C8-N9-C4	5.15	107.86	105.80
1	AA	1016	A	N9-C4-C5	5.15	107.86	105.80
33	BA	477	A	C8-N9-C4	5.14	107.86	105.80
33	BA	1615	A	N9-C4-C5	5.14	107.86	105.80
33	BA	1506	A	C8-N9-C4	5.14	107.86	105.80
33	BA	2663	A	C5-C6-N1	5.14	120.27	117.70
33	BA	61	A	N9-C4-C5	5.14	107.86	105.80
33	BA	1919	A	C4-C5-C6	5.14	119.57	117.00
1	AA	128	A	N9-C4-C5	5.14	107.86	105.80
1	AA	457	A	C8-N9-C4	5.14	107.86	105.80
1	AA	1234	A	N9-C4-C5	5.14	107.86	105.80
1	AA	1442	A	N9-C4-C5	5.14	107.86	105.80
1	AA	496	A	N9-C4-C5	5.14	107.86	105.80
33	BA	118	A	C4-C5-N7	-5.14	108.13	110.70
33	BA	2916	A	C5-C6-N1	5.14	120.27	117.70
1	AA	301	A	N9-C4-C5	5.14	107.85	105.80
1	AA	727	A	C8-N9-C4	5.14	107.86	105.80
1	AA	874	A	N9-C4-C5	5.14	107.86	105.80
33	BA	527	A	C8-N9-C4	5.14	107.86	105.80
33	BA	1131	A	N9-C4-C5	5.14	107.86	105.80
33	BA	2296	A	C8-N9-C4	5.14	107.86	105.80
34	BB	51	A	N9-C4-C5	5.14	107.85	105.80
33	BA	462	A	C4-C5-N7	-5.13	108.13	110.70
33	BA	1243	A	C5-C6-N1	5.13	120.27	117.70
33	BA	1695	A	N9-C4-C5	5.13	107.85	105.80
33	BA	2805	A	N9-C4-C5	5.13	107.85	105.80
33	BA	2812	A	N9-C4-C5	5.13	107.85	105.80
33	BA	2851	A	N9-C4-C5	5.13	107.85	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	462	A	N9-C4-C5	5.13	107.85	105.80
33	BA	1100	A	N9-C4-C5	5.13	107.85	105.80
33	BA	41	A	N9-C4-C5	5.13	107.85	105.80
33	BA	2117	A	C4-C5-N7	-5.13	108.14	110.70
33	BA	1858	A	N9-C4-C5	5.13	107.85	105.80
1	AA	811	A	N9-C4-C5	5.13	107.85	105.80
1	AA	1238	A	C4-C5-N7	-5.13	108.14	110.70
1	AA	1296	A	N9-C4-C5	5.13	107.85	105.80
33	BA	52	A	C8-N9-C4	5.13	107.85	105.80
33	BA	407	A	C5-C6-N1	5.13	120.27	117.70
33	BA	1006	A	N9-C4-C5	5.13	107.85	105.80
33	BA	2844	A	N9-C4-C5	5.13	107.85	105.80
33	BA	2885	A	C4-C5-N7	-5.13	108.14	110.70
33	BA	2148	A	N9-C4-C5	5.13	107.85	105.80
33	BA	2500	A	C5-C6-N1	5.13	120.26	117.70
33	BA	1316	A	C5-C6-N1	5.12	120.26	117.70
33	BA	1524	A	C5-C6-N1	5.12	120.26	117.70
1	AA	1358	A	C4-C5-C6	5.12	119.56	117.00
33	BA	1569	A	N9-C4-C5	5.12	107.85	105.80
1	AA	391	A	C8-N9-C4	5.12	107.85	105.80
1	AA	1256	A	C4-C5-N7	-5.12	108.14	110.70
33	BA	1905	A	C4-C5-C6	5.12	119.56	117.00
33	BA	2026	A	N9-C4-C5	5.12	107.85	105.80
33	BA	2227	A	N9-C4-C5	5.12	107.85	105.80
1	AA	1294	A	N9-C4-C5	5.12	107.85	105.80
33	BA	374	A	C5-C6-N1	5.12	120.26	117.70
1	AA	987	A	C4-C5-N7	-5.12	108.14	110.70
33	BA	1006	A	C4-C5-N7	-5.12	108.14	110.70
33	BA	1620	A	C4-C5-N7	-5.12	108.14	110.70
33	BA	1925	A	N9-C4-C5	5.12	107.85	105.80
33	BA	2898	A	C5-C6-N1	5.12	120.26	117.70
33	BA	870	A	C5-C6-N1	5.12	120.26	117.70
33	BA	1042	A	N9-C4-C5	5.12	107.85	105.80
1	AA	391	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	397	A	N9-C4-C5	5.12	107.85	105.80
1	AA	993	A	C5-C6-N1	5.12	120.26	117.70
33	BA	908	A	C8-N9-C4	5.12	107.85	105.80
1	AA	605	A	N9-C4-C5	5.11	107.84	105.80
1	AA	1369	A	C5-C6-N1	5.11	120.26	117.70
33	BA	1858	A	C4-C5-N7	-5.11	108.14	110.70
1	AA	948	A	C4-C5-N7	-5.11	108.14	110.70
33	BA	647	A	C5-C6-N1	5.11	120.26	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1424	A	N9-C4-C5	5.11	107.84	105.80
33	BA	1606	A	C4-C5-N7	-5.11	108.15	110.70
33	BA	2593	A	C8-N9-C4	5.11	107.84	105.80
1	AA	74	A	C5-C6-N1	5.11	120.25	117.70
1	AA	993	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	1155	A	C8-N9-C4	5.11	107.84	105.80
33	BA	1357	A	C5-C6-N1	5.11	120.25	117.70
33	BA	1831	A	N9-C4-C5	5.11	107.84	105.80
33	BA	1883	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	948	A	N9-C4-C5	5.11	107.84	105.80
1	AA	1026	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	1188	A	C5-C6-N1	5.11	120.25	117.70
21	AX	9	A	N9-C4-C5	5.11	107.84	105.80
33	BA	374	A	N3-C4-N9	5.11	131.49	127.40
33	BA	849	A	C8-N9-C4	5.11	107.84	105.80
33	BA	2254	A	C5-C6-N1	5.11	120.25	117.70
33	BA	2365	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	1358	A	C4-C5-N7	-5.10	108.15	110.70
33	BA	673	A	C4-C5-N7	-5.10	108.15	110.70
33	BA	1520	A	C4-C5-N7	-5.10	108.15	110.70
33	BA	1691	A	C5-C6-N1	5.10	120.25	117.70
33	BA	2357	A	C8-N9-C4	5.10	107.84	105.80
1	AA	1238	A	N9-C4-C5	5.10	107.84	105.80
33	BA	1194	A	N9-C4-C5	5.10	107.84	105.80
33	BA	1480	A	N9-C4-C5	5.10	107.84	105.80
33	BA	2358	A	C8-N9-C4	5.10	107.84	105.80
33	BA	2778	A	C8-N9-C4	5.10	107.84	105.80
33	BA	1648	A	N9-C4-C5	5.10	107.84	105.80
34	BB	20	A	C4-C5-N7	-5.10	108.15	110.70
1	AA	617	A	C5-C6-N1	5.10	120.25	117.70
1	AA	996	A	C4-C5-N7	-5.10	108.15	110.70
21	AX	24	A	C4-C5-N7	-5.10	108.15	110.70
33	BA	268	A	C8-N9-C4	5.10	107.84	105.80
33	BA	2407	A	C4-C5-N7	-5.10	108.15	110.70
33	BA	2662	A	C5-C6-N1	5.10	120.25	117.70
33	BA	1883	A	N9-C4-C5	5.10	107.84	105.80
34	BB	97	A	N9-C4-C5	5.10	107.84	105.80
33	BA	574	A	C5-C6-N1	5.09	120.25	117.70
33	BA	964	A	N9-C4-C5	5.09	107.84	105.80
33	BA	1672	A	N9-C4-C5	5.09	107.84	105.80
33	BA	2080	A	N9-C4-C5	5.09	107.84	105.80
1	AA	433	A	C5-C6-N1	5.09	120.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	1709	A	N9-C4-C5	5.09	107.84	105.80
1	AA	1355	A	C4-C5-C6	5.09	119.55	117.00
33	BA	690	A	C5-C6-N1	5.09	120.25	117.70
33	BA	2143	A	C4-C5-N7	-5.09	108.15	110.70
33	BA	2200	A	N9-C4-C5	5.09	107.84	105.80
1	AA	1490	A	C5-C6-N1	5.09	120.25	117.70
33	BA	305	A	N9-C4-C5	5.09	107.84	105.80
33	BA	517	A	N9-C4-C5	5.09	107.84	105.80
33	BA	1928	A	C5-C6-N1	5.09	120.25	117.70
33	BA	2111	A	C4-C5-N7	-5.09	108.16	110.70
1	AA	114	A	N9-C4-C5	5.09	107.83	105.80
1	AA	346	A	N9-C4-C5	5.09	107.83	105.80
33	BA	133	A	C5-C6-N1	5.09	120.24	117.70
1	AA	996	A	N9-C4-C5	5.09	107.83	105.80
33	BA	281	A	C5-C6-N1	5.09	120.24	117.70
33	BA	1190	A	C5-C6-N1	5.09	120.24	117.70
33	BA	1888	A	N9-C4-C5	5.09	107.83	105.80
33	BA	2454	A	N9-C4-C5	5.09	107.83	105.80
1	AA	945	A	C5-C6-N1	5.08	120.24	117.70
33	BA	374	A	C4-C5-C6	5.08	119.54	117.00
33	BA	656	A	N9-C4-C5	5.08	107.83	105.80
1	AA	439	A	C8-N9-C4	5.08	107.83	105.80
33	BA	171	A	N9-C4-C5	5.08	107.83	105.80
33	BA	1316	A	N9-C4-C5	5.08	107.83	105.80
1	AA	1278	A	C4-C5-N7	-5.08	108.16	110.70
33	BA	44	A	C5-C6-N1	5.08	120.24	117.70
33	BA	1700	A	C5-C6-N1	5.08	120.24	117.70
1	AA	1366	A	C4-C5-N7	-5.08	108.16	110.70
33	BA	1253	A	N9-C4-C5	5.08	107.83	105.80
33	BA	894	A	C8-N9-C4	5.08	107.83	105.80
1	AA	1517	A	C5-C6-N1	5.08	120.24	117.70
33	BA	525	A	C5-C6-N1	5.08	120.24	117.70
33	BA	1074	A	C5-C6-N1	5.08	120.24	117.70
33	BA	1284	A	N9-C4-C5	5.08	107.83	105.80
33	BA	1774	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	278	A	N9-C4-C5	5.07	107.83	105.80
1	AA	1349	A	C5-C6-N1	5.07	120.24	117.70
33	BA	1194	A	C5-C6-N1	5.07	120.24	117.70
33	BA	1442	A	C4-C5-N7	-5.07	108.16	110.70
33	BA	2691	A	C4-C5-N7	-5.07	108.16	110.70
1	AA	1143	A	N9-C4-C5	5.07	107.83	105.80
33	BA	692	A	N9-C4-C5	5.07	107.83	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1160	A	N9-C4-C5	5.07	107.83	105.80
33	BA	2123	A	N9-C4-C5	5.07	107.83	105.80
34	BB	25	A	N9-C4-C5	5.07	107.83	105.80
33	BA	1067	A	C4-C5-N7	-5.07	108.17	110.70
33	BA	2270	A	C5-C6-N1	5.07	120.23	117.70
1	AA	883	A	N9-C4-C5	5.07	107.83	105.80
33	BA	1814	A	C5-C6-N1	5.07	120.23	117.70
33	BA	2663	A	N9-C4-C5	5.07	107.83	105.80
33	BA	2689	A	C8-N9-C4	5.07	107.83	105.80
33	BA	2694	A	N9-C4-C5	5.07	107.83	105.80
1	AA	405	A	C8-N9-C4	5.06	107.83	105.80
33	BA	870	A	N9-C4-C5	5.06	107.83	105.80
33	BA	1491	A	C8-N9-C4	5.06	107.83	105.80
1	AA	278	A	C5-C6-N1	5.06	120.23	117.70
1	AA	301	A	C5-C6-N1	5.06	120.23	117.70
1	AA	1341	A	C8-N9-C4	5.06	107.83	105.80
33	BA	496	A	N9-C4-C5	5.06	107.83	105.80
33	BA	656	A	C5-C6-N1	5.06	120.23	117.70
33	BA	715	A	N9-C4-C5	5.06	107.83	105.80
33	BA	1188	A	C4-C5-N7	-5.06	108.17	110.70
33	BA	1258	A	N9-C4-C5	5.06	107.83	105.80
33	BA	2381	A	N9-C4-C5	5.06	107.83	105.80
33	BA	1222	A	N9-C4-C5	5.06	107.82	105.80
33	BA	2436	A	C4-C5-N7	-5.06	108.17	110.70
1	AA	1435	A	C5-C6-N1	5.05	120.23	117.70
33	BA	526	A	N3-C4-N9	5.05	131.44	127.40
33	BA	1132	A	C8-N9-C4	5.05	107.82	105.80
33	BA	1700	A	N9-C4-C5	5.05	107.82	105.80
33	BA	2091	A	C8-N9-C4	5.05	107.82	105.80
33	BA	2351	A	C5-C6-N1	5.05	120.23	117.70
1	AA	361	A	N9-C4-C5	5.05	107.82	105.80
33	BA	130	A	C5-C6-N1	5.05	120.23	117.70
33	BA	1305	A	C4-C5-C6	5.05	119.53	117.00
33	BA	1562	A	C5-C6-N1	5.05	120.23	117.70
33	BA	1820	A	C8-N9-C4	5.05	107.82	105.80
33	BA	2719	A	C5-C6-N1	5.05	120.23	117.70
33	BA	2722	A	C5-C6-N1	5.05	120.23	117.70
33	BA	661	A	C4-C5-N7	-5.05	108.17	110.70
33	BA	1126	A	N9-C4-C5	5.05	107.82	105.80
33	BA	1244	A	C5-C6-N1	5.05	120.22	117.70
33	BA	1667	A	C4-C5-N7	-5.05	108.18	110.70
33	BA	2205	A	C5-C6-N1	5.05	120.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BA	2790	A	N9-C4-C5	5.05	107.82	105.80
1	AA	721	A	C5-C6-N1	5.05	120.22	117.70
1	AA	1188	A	N9-C4-C5	5.05	107.82	105.80
33	BA	1562	A	C8-N9-C4	5.05	107.82	105.80
33	BA	2027	A	C5-C6-N1	5.05	120.22	117.70
1	AA	882	A	C4-C5-N7	-5.05	108.18	110.70
1	AA	987	A	N9-C4-C5	5.05	107.82	105.80
33	BA	1222	A	C5-C6-N1	5.05	120.22	117.70
33	BA	1858	A	C5-C6-N1	5.05	120.22	117.70
33	BA	2042	A	C5-C6-N1	5.05	120.22	117.70
33	BA	830	A	C8-N9-C4	5.04	107.82	105.80
1	AA	875	A	C4-C5-N7	-5.04	108.18	110.70
33	BA	2123	A	C4-C5-N7	-5.04	108.18	110.70
33	BA	2358	A	C4-C5-N7	-5.04	108.18	110.70
1	AA	674	A	C5-C6-N1	5.04	120.22	117.70
33	BA	1067	A	N3-C4-N9	5.04	131.43	127.40
1	AA	649	A	N9-C4-C5	5.04	107.82	105.80
1	AA	72	A	C5-C6-N1	5.04	120.22	117.70
1	AA	631	A	C5-C6-N1	5.04	120.22	117.70
1	AA	838	A	N9-C4-C5	5.04	107.82	105.80
1	AA	1245	A	N9-C4-C5	5.04	107.82	105.80
33	BA	438	A	C5-C6-N1	5.04	120.22	117.70
33	BA	689	A	N9-C4-C5	5.04	107.82	105.80
33	BA	1620	A	N9-C4-C5	5.04	107.81	105.80
33	BA	2241	A	N3-C4-N9	5.04	131.43	127.40
33	BA	2627	A	C4-C5-N7	-5.04	108.18	110.70
1	AA	775	A	C5-C6-N1	5.04	120.22	117.70
33	BA	722	A	N9-C4-C5	5.04	107.81	105.80
33	BA	156	A	N9-C4-C5	5.04	107.81	105.80
33	BA	1998	A	N9-C4-C5	5.04	107.81	105.80
34	BB	46	A	N9-C4-C5	5.04	107.81	105.80
1	AA	548	A	N9-C4-C5	5.03	107.81	105.80
1	AA	650	A	N9-C4-C5	5.03	107.81	105.80
1	AA	1022	A	C5-C6-N1	5.03	120.22	117.70
1	AA	948	A	C5-C6-N1	5.03	120.22	117.70
1	AA	956	A	C5-C6-N1	5.03	120.22	117.70
33	BA	882	A	N9-C4-C5	5.03	107.81	105.80
33	BA	1839	A	N9-C4-C5	5.03	107.81	105.80
47	BR	22	LEU	CA-CB-CG	5.03	126.87	115.30
33	BA	183	A	N3-C4-N9	5.03	131.42	127.40
33	BA	1477	A	N9-C4-C5	5.03	107.81	105.80
33	BA	2043	A	N9-C4-C5	5.03	107.81	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	151	A	C5-C6-N1	5.03	120.21	117.70
1	AA	899	A	C5-C6-N1	5.03	120.21	117.70
1	AA	933	A	C4-C5-N7	-5.03	108.19	110.70
1	AA	1372	A	C5-C6-N1	5.03	120.21	117.70
33	BA	326	A	C5-C6-N1	5.02	120.21	117.70
1	AA	862	A	N3-C4-N9	5.02	131.42	127.40
33	BA	28	A	C5-C6-N1	5.02	120.21	117.70
33	BA	525	A	C4-C5-N7	-5.02	108.19	110.70
33	BA	724	A	C5-C6-N1	5.02	120.21	117.70
1	AA	696	A	N9-C4-C5	5.02	107.81	105.80
1	AA	1272	A	N9-C4-C5	5.02	107.81	105.80
33	BA	462	A	C5-C6-N1	5.02	120.21	117.70
33	BA	970	A	N9-C4-C5	5.02	107.81	105.80
33	BA	1473	A	C5-C6-N1	5.02	120.21	117.70
33	BA	2220	A	C5-C6-N1	5.02	120.21	117.70
33	BA	53	A	C5-C6-N1	5.02	120.21	117.70
1	AA	548	A	C4-C5-N7	-5.02	108.19	110.70
1	AA	1355	A	C5-C6-N1	5.02	120.21	117.70
21	AX	24	A	N9-C4-C5	5.02	107.81	105.80
33	BA	2459	A	N9-C4-C5	5.02	107.81	105.80
33	BA	1714	A	C8-N9-C4	5.01	107.81	105.80
1	AA	664	A	C5-C6-N1	5.01	120.21	117.70
33	BA	1103	A	C4-C5-N7	-5.01	108.19	110.70
1	AA	1384	A	N9-C4-C5	5.01	107.81	105.80
33	BA	956	A	C5-C6-N1	5.01	120.21	117.70
33	BA	2447	A	C5-C6-N1	5.01	120.21	117.70
33	BA	2907	A	C5-C6-N1	5.01	120.20	117.70
1	AA	55	A	C5-C6-N1	5.01	120.20	117.70
33	BA	108	A	N9-C4-C5	5.01	107.80	105.80
1	AA	715	A	C5-C6-N1	5.01	120.20	117.70
33	BA	1999	A	N9-C4-C5	5.01	107.80	105.80
1	AA	1288	A	N9-C4-C5	5.00	107.80	105.80
33	BA	6	A	C5-C6-N1	5.00	120.20	117.70
33	BA	910	A	C4-C5-N7	-5.00	108.20	110.70
33	BA	1412	A	C5-C6-N1	5.00	120.20	117.70
33	BA	1776	A	C5-C6-N1	5.00	120.20	117.70
33	BA	178	A	C8-N9-C4	5.00	107.80	105.80
33	BA	307	A	C5-C6-N1	5.00	120.20	117.70
33	BA	736	A	C4-C5-N7	-5.00	108.20	110.70
33	BA	1930	A	C5-C6-N1	5.00	120.20	117.70
33	BA	2468	A	C4-C5-N7	-5.00	108.20	110.70
33	BA	2793	A	C5-C6-N1	5.00	120.20	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BB	13	A	C4-C5-N7	-5.00	108.20	110.70

There are no chirality outliers.

All (134) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1026	A	Sidechain
1	AA	1065	A	Sidechain
1	AA	1207	A	Sidechain
1	AA	1261	A	Sidechain
1	AA	1278	A	Sidechain
1	AA	1294	A	Sidechain
1	AA	1297	A	Sidechain
1	AA	1384	A	Sidechain
1	AA	1407	A	Sidechain
1	AA	1427	A	Sidechain
1	AA	1442	A	Sidechain
1	AA	1478	A	Sidechain
1	AA	209	A	Sidechain
1	AA	308	A	Sidechain
1	AA	335	A	Sidechain
1	AA	391	A	Sidechain
1	AA	401	A	Sidechain
1	AA	415	A	Sidechain
1	AA	419	A	Sidechain
1	AA	496	A	Sidechain
1	AA	500	A	Sidechain
1	AA	53	A	Sidechain
1	AA	532	A	Sidechain
1	AA	583	A	Sidechain
1	AA	696	A	Sidechain
1	AA	76	A	Sidechain
1	AA	790	A	Sidechain
1	AA	811	A	Sidechain
1	AA	862	A	Sidechain
1	AA	879	A	Sidechain
1	AA	883	A	Sidechain
1	AA	911	A	Sidechain
1	AA	918	A	Sidechain
1	AA	969	A	Sidechain
1	AA	975	A	Sidechain
1	AA	988	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AX	37	A	Sidechain
21	AX	9	A	Sidechain
22	AY	12	A	Sidechain
22	AY	15	A	Sidechain
22	AY	16	A	Sidechain
22	AY	18	A	Sidechain
22	AY	5	A	Sidechain
22	AY	6	A	Sidechain
22	AY	9	A	Sidechain
33	BA	1006	A	Sidechain
33	BA	1042	A	Sidechain
33	BA	1075	A	Sidechain
33	BA	1078	A	Sidechain
33	BA	1094	A	Sidechain
33	BA	1097	A	Sidechain
33	BA	1172	A	Sidechain
33	BA	1173	A	Sidechain
33	BA	1253	A	Sidechain
33	BA	126	A	Sidechain
33	BA	1293	A	Sidechain
33	BA	1294	A	Sidechain
33	BA	1302	A	Sidechain
33	BA	1393	A	Sidechain
33	BA	1555	A	Sidechain
33	BA	1618	A	Sidechain
33	BA	1619	A	Sidechain
33	BA	1659	A	Sidechain
33	BA	1661	A	Sidechain
33	BA	168	A	Sidechain
33	BA	1686	A	Sidechain
33	BA	1724	A	Sidechain
33	BA	183	A	Sidechain
33	BA	1831	A	Sidechain
33	BA	1839	A	Sidechain
33	BA	1883	A	Sidechain
33	BA	1888	A	Sidechain
33	BA	1957	A	Sidechain
33	BA	1998	A	Sidechain
33	BA	2006	A	Sidechain
33	BA	2010	A	Sidechain
33	BA	2043	A	Sidechain
33	BA	2062	A	Sidechain

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Mol	Chain	Res	Type	Group
33	BA	2111	A	Sidechain
33	BA	2164	A	Sidechain
33	BA	2176	A	Sidechain
33	BA	2241	A	Sidechain
33	BA	2262	A	Sidechain
33	BA	2316	A	Sidechain
33	BA	2364	A	Sidechain
33	BA	2383	A	Sidechain
33	BA	2395	A	Sidechain
33	BA	2407	A	Sidechain
33	BA	2488	A	Sidechain
33	BA	259	A	Sidechain
33	BA	2601	A	Sidechain
33	BA	2606	A	Sidechain
33	BA	2616	A	Sidechain
33	BA	2627	A	Sidechain
33	BA	2631	A	Sidechain
33	BA	2670	A	Sidechain
33	BA	2691	A	Sidechain
33	BA	2708	A	Sidechain
33	BA	2805	A	Sidechain
33	BA	2819	A	Sidechain
33	BA	2827	A	Sidechain
33	BA	2885	A	Sidechain
33	BA	366	A	Sidechain
33	BA	477	A	Sidechain
33	BA	501	A	Sidechain
33	BA	513	A	Sidechain
33	BA	517	A	Sidechain
33	BA	518	A	Sidechain
33	BA	52	A	Sidechain
33	BA	538	A	Sidechain
33	BA	551	A	Sidechain
33	BA	559	A	Sidechain
33	BA	64	A	Sidechain
33	BA	661	A	Sidechain
33	BA	67	A	Sidechain
33	BA	679	A	Sidechain
33	BA	692	A	Sidechain
33	BA	699	A	Sidechain
33	BA	722	A	Sidechain
33	BA	752	A	Sidechain

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Mol	Chain	Res	Type	Group
33	BA	765	A	Sidechain
33	BA	796	A	Sidechain
33	BA	797	A	Sidechain
33	BA	798	A	Sidechain
33	BA	799	A	Sidechain
33	BA	836	A	Sidechain
33	BA	841	A	Sidechain
33	BA	866	A	Sidechain
33	BA	904	A	Sidechain
34	BB	55	A	Sidechain
34	BB	97	A	Sidechain
37	BF	66	ARG	Sidechain
51	BV	86	ARG	Sidechain
51	BV	88	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33115	0	16676	250	0
2	AB	896	0	244	2	0
3	AC	840	0	241	3	0
4	AD	797	0	224	3	0
5	AE	661	0	197	1	0
6	AF	381	0	104	0	0
7	AG	613	0	164	1	0
8	AH	525	0	146	0	0
9	AI	521	0	155	4	0
10	AJ	409	0	104	0	0
11	AK	472	0	135	7	0
12	AL	549	0	157	1	0
13	AM	476	0	137	2	0
14	AN	241	0	62	2	0
15	AO	353	0	94	0	0
16	AP	357	0	95	0	0
17	AQ	345	0	90	1	0
18	AR	285	0	76	1	0
19	AS	336	0	93	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	AT	345	0	89	2	0
21	AX	1643	0	830	30	0
22	AY	415	0	207	80	0
23	AZ	107	0	58	9	0
24	B0	444	0	486	61	0
25	B1	530	0	568	12	0
26	B2	455	0	491	12	0
27	B3	503	0	494	12	0
28	B4	426	0	445	14	0
29	B5	401	0	413	18	0
30	B6	367	0	410	20	0
31	B7	512	0	564	31	0
32	B8	288	0	330	3	0
33	BA	62767	0	31584	776	0
34	BB	2395	0	1212	21	0
35	BD	2111	0	2200	85	0
36	BE	1575	0	1642	48	0
37	BF	1561	0	1647	92	0
38	BG	1404	0	1467	44	0
39	BH	1342	0	1388	26	0
40	BJ	955	0	990	24	0
41	BK	981	0	1020	27	0
42	BM	1123	0	1162	31	0
43	BN	920	0	977	21	0
44	BO	1081	0	1132	40	0
45	BP	1097	0	1165	25	0
46	BQ	953	0	983	28	0
47	BR	912	0	947	36	0
48	BS	936	0	1008	31	0
49	BT	940	0	1005	41	0
50	BU	786	0	826	40	0
51	BV	842	0	899	46	0
52	BW	752	0	802	19	0
53	BX	754	0	809	31	0
54	BZ	630	0	644	16	0
All	All	135425	0	80088	1864	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 9.

All (1864) 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)
23:AZ:74:ILE:CA	51:BV:85:PHE:HE2	1.11	1.60
23:AZ:74:ILE:CA	51:BV:85:PHE:CE2	1.99	1.44
24:B0:37:ARG:NH1	24:B0:44:PRO:HG3	1.37	1.40
37:BF:80:SER:OG	37:BF:81:PRO:HD2	1.30	1.29
41:BK:15:ALA:HB1	41:BK:46:THR:CG2	1.62	1.28
24:B0:37:ARG:HD2	24:B0:44:PRO:CB	1.65	1.24
22:AY:4:G:H2'	22:AY:5:A:H5'	1.21	1.18
47:BR:64:ASN:HB3	47:BR:66:GLU:HG2	1.23	1.14
41:BK:15:ALA:CB	41:BK:46:THR:CG2	2.26	1.14
41:BK:15:ALA:CB	41:BK:46:THR:HG21	1.79	1.12
53:BX:87:ASP:HB3	53:BX:88:GLY:HA3	1.31	1.12
24:B0:38:ILE:HD11	24:B0:49:VAL:HB	1.30	1.11
33:BA:374:A:C2	33:BA:1250:G:H2'	1.84	1.11
41:BK:46:THR:HG23	41:BK:54:ILE:HD12	1.31	1.11
41:BK:15:ALA:HB1	41:BK:46:THR:HG22	1.14	1.10
24:B0:37:ARG:HD3	24:B0:45:LYS:CG	1.83	1.09
22:AY:4:G:C2'	22:AY:5:A:H5'	1.83	1.08
47:BR:22:LEU:HD22	47:BR:94:VAL:HG11	1.34	1.08
24:B0:37:ARG:HD2	24:B0:44:PRO:HB2	1.08	1.07
30:B6:34:ARG:HG2	30:B6:42:LEU:HD12	1.28	1.06
39:BH:21:ASP:HB3	39:BH:22:ASN:HB2	1.36	1.05
24:B0:37:ARG:CD	24:B0:44:PRO:HB2	1.86	1.05
24:B0:45:LYS:HB3	24:B0:46:LYS:HB2	1.37	1.03
37:BF:77:SER:HB2	37:BF:80:SER:HB2	1.40	1.02
37:BF:80:SER:HB3	37:BF:83:TRP:HD1	1.23	1.02
33:BA:377:G:H2'	33:BA:378:C:C6	1.94	1.02
30:B6:34:ARG:HG2	30:B6:42:LEU:CD1	1.91	1.00
33:BA:377:G:H2'	33:BA:378:C:H6	1.22	1.00
33:BA:924:U:H3	33:BA:946:G:H1	1.10	1.00
37:BF:66:ARG:HH11	37:BF:70:THR:CG2	1.76	0.98
33:BA:1264:G:H4'	50:BU:87:GLY:O	1.63	0.98
33:BA:1024:G:H1	33:BA:1031:C:N4	1.61	0.98
24:B0:37:ARG:HG3	24:B0:45:LYS:HG2	1.46	0.98
24:B0:37:ARG:CG	24:B0:45:LYS:HG2	1.95	0.96
37:BF:65:TRP:CZ2	37:BF:75:GLN:HB2	2.00	0.96
24:B0:37:ARG:HH11	24:B0:44:PRO:CG	1.78	0.96
24:B0:37:ARG:CD	24:B0:45:LYS:HG2	1.94	0.96
33:BA:1353:C:H42	33:BA:1377:G:H1	0.97	0.95
24:B0:45:LYS:HB3	24:B0:46:LYS:CB	1.95	0.95
24:B0:37:ARG:CD	24:B0:45:LYS:CG	2.44	0.95
33:BA:2009:G:C6	33:BA:2011:U:C4	2.55	0.95
33:BA:528:G:H1	33:BA:555:C:N4	1.63	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:774:G:H1	1:AA:821:G:HO2'	1.15	0.94
22:AY:2:G:H2'	22:AY:2:G:N3	1.84	0.93
1:AA:1551:U:H3	22:AY:2:G:H22	1.07	0.92
37:BF:73:ALA:HB3	37:BF:75:GLN:HG2	1.49	0.92
33:BA:2799:C:C5	33:BA:2800:C:C5	2.58	0.91
24:B0:37:ARG:HB2	24:B0:45:LYS:HD3	1.51	0.91
33:BA:1295:U:C4	37:BF:72:ARG:O	2.23	0.91
37:BF:65:TRP:CZ2	37:BF:75:GLN:CB	2.54	0.90
33:BA:796:A:H61	33:BA:800:G:H21	1.19	0.90
37:BF:66:ARG:HH11	37:BF:70:THR:HG22	1.33	0.90
37:BF:75:GLN:HE22	37:BF:82:GLN:NE2	1.68	0.90
33:BA:797:A:C2	33:BA:799:A:H5'	2.07	0.90
33:BA:1024:G:H1	33:BA:1031:C:H42	1.04	0.90
35:BD:243:ARG:HH22	35:BD:247:MET:CB	1.85	0.90
11:AK:38:ASP:O	11:AK:41:GLY:CA	2.19	0.89
33:BA:1364:C:C2	51:BV:86:ARG:CZ	2.56	0.89
24:B0:37:ARG:HD2	24:B0:44:PRO:CG	2.02	0.89
50:BU:67:ARG:HH11	50:BU:89:ARG:NH1	1.69	0.89
37:BF:75:GLN:NE2	37:BF:82:GLN:NE2	2.21	0.88
33:BA:609:C:OP2	50:BU:79:LYS:HD3	1.73	0.88
22:AY:3:U:H2'	22:AY:4:G:C8	2.09	0.88
11:AK:40:HIS:N	11:AK:41:GLY:HA2	1.87	0.88
33:BA:2089:A:H3'	37:BF:68:LYS:HE2	1.56	0.88
24:B0:40:VAL:HG12	24:B0:41:ASN:H	1.36	0.88
33:BA:528:G:H1	33:BA:555:C:H42	0.87	0.87
53:BX:87:ASP:CB	53:BX:88:GLY:HA3	2.04	0.87
37:BF:66:ARG:NH1	37:BF:70:THR:HG22	1.88	0.87
30:B6:34:ARG:CG	30:B6:42:LEU:CD1	2.53	0.87
47:BR:64:ASN:CB	47:BR:66:GLU:HG2	2.04	0.86
33:BA:1353:C:N4	33:BA:1377:G:H1	1.71	0.86
49:BT:103:LEU:HD12	49:BT:104:THR:HA	1.55	0.86
22:AY:5:A:H2'	22:AY:6:A:H5''	1.56	0.86
47:BR:65:VAL:CG1	47:BR:73:ALA:HB1	2.06	0.85
37:BF:80:SER:OG	37:BF:81:PRO:CD	2.21	0.85
33:BA:2355:U:H3	33:BA:2418:G:H1	1.24	0.85
1:AA:732:U:C4	22:AY:7:C:O2'	2.30	0.85
11:AK:38:ASP:O	11:AK:41:GLY:HA3	1.76	0.84
22:AY:1:U:H2'	22:AY:2:G:H1'	1.58	0.84
33:BA:1294:A:H3'	33:BA:1295:U:H5''	1.60	0.84
47:BR:22:LEU:CD2	47:BR:94:VAL:HG11	2.08	0.83
37:BF:62:ARG:O	37:BF:78:ILE:HG13	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AX:74:C:H5'	33:BA:2631:A:H5''	1.58	0.82
47:BR:22:LEU:HD22	47:BR:94:VAL:CG1	2.09	0.82
22:AY:5:A:C2	22:AY:6:A:H1'	2.15	0.82
33:BA:2089:A:H3'	37:BF:68:LYS:CE	2.10	0.82
44:BO:117:LEU:HA	44:BO:118:GLU:HB3	1.60	0.82
33:BA:1711:G:H1	33:BA:2023:C:H42	1.24	0.82
24:B0:45:LYS:HB3	24:B0:46:LYS:CA	2.09	0.81
22:AY:10:U:O2'	22:AY:11:G:C4	2.32	0.81
21:AX:72:C:H6	21:AX:72:C:H5''	1.43	0.81
51:BV:88:ARG:HD2	51:BV:94:SER:OG	1.79	0.81
1:AA:268:G:N2	1:AA:273:G:N7	2.29	0.81
33:BA:1656:C:O2'	33:BA:1657:C:H5'	1.80	0.80
30:B6:34:ARG:CG	30:B6:42:LEU:HD13	2.11	0.80
26:B2:11:SER:HB2	33:BA:1034:A:H5''	1.63	0.80
1:AA:964:G:H21	1:AA:1236:A:H62	1.30	0.80
33:BA:1297:C:H5'	37:BF:75:GLN:OE1	1.81	0.80
24:B0:37:ARG:HH11	24:B0:44:PRO:HG3	0.98	0.80
41:BK:46:THR:CG2	41:BK:54:ILE:HD12	2.10	0.80
33:BA:2009:G:C5	33:BA:2011:U:C5	2.69	0.80
51:BV:82:LEU:HB2	51:BV:98:LYS:HB2	1.62	0.80
24:B0:37:ARG:HD3	24:B0:45:LYS:HG3	1.64	0.79
33:BA:2799:C:H5	33:BA:2800:C:C5	1.98	0.79
33:BA:1834:C:H42	33:BA:1841:G:H1	1.30	0.79
33:BA:15:G:H1	33:BA:571:U:H3	1.29	0.79
24:B0:45:LYS:CB	24:B0:46:LYS:HB2	2.11	0.79
37:BF:62:ARG:O	37:BF:78:ILE:CG1	2.30	0.79
47:BR:65:VAL:CG1	47:BR:73:ALA:CB	2.60	0.79
22:AY:5:A:C4	22:AY:6:A:C8	2.69	0.79
33:BA:2799:C:H5	33:BA:2800:C:H5	1.29	0.78
41:BK:46:THR:HG23	41:BK:54:ILE:CD1	2.11	0.78
24:B0:37:ARG:HD3	24:B0:45:LYS:CD	2.14	0.78
37:BF:80:SER:HB3	37:BF:83:TRP:CD1	2.14	0.78
33:BA:364:A:H4'	33:BA:366:A:C8	2.18	0.77
51:BV:89:ALA:O	51:BV:90:MET:HB2	1.84	0.77
33:BA:1263:G:C5	50:BU:70:LYS:NZ	2.52	0.77
33:BA:1103:A:N6	33:BA:1133:G:OP2	2.17	0.77
33:BA:2799:C:C5	33:BA:2800:C:H5	1.99	0.77
1:AA:1546:C:H2'	1:AA:1547:U:C6	2.19	0.77
37:BF:65:TRP:HZ2	37:BF:75:GLN:CB	1.98	0.77
24:B0:37:ARG:CD	24:B0:44:PRO:CB	2.54	0.77
1:AA:1323:C:H42	1:AA:1332:G:H1	1.29	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:2799:C:H5'	33:BA:2800:C:OP2	1.85	0.76
24:B0:37:ARG:HB2	24:B0:45:LYS:CD	2.14	0.76
41:BK:15:ALA:HB2	41:BK:46:THR:HG21	1.67	0.76
28:B4:50:ASN:ND2	33:BA:2909:U:O2	2.18	0.76
33:BA:528:G:N2	33:BA:555:C:N3	2.33	0.76
24:B0:37:ARG:NH1	24:B0:44:PRO:CG	2.33	0.76
33:BA:1294:A:H3'	33:BA:1295:U:C5'	2.16	0.75
29:B5:21:LYS:HD3	33:BA:2315:A:H62	1.51	0.75
37:BF:80:SER:HG	37:BF:81:PRO:HD2	1.51	0.75
33:BA:797:A:H2	33:BA:799:A:H5'	1.48	0.75
33:BA:426:G:H1	33:BA:442:C:H42	1.35	0.75
47:BR:65:VAL:HG11	47:BR:73:ALA:CB	2.17	0.74
33:BA:374:A:N1	33:BA:1250:G:H2'	2.01	0.74
30:B6:31:LEU:CD2	30:B6:42:LEU:HD11	2.17	0.74
33:BA:775:G:H5'	35:BD:13:ARG:HH21	1.52	0.74
35:BD:243:ARG:NH2	35:BD:247:MET:HB3	2.01	0.74
33:BA:1659:A:H2	51:BV:93:ALA:HB2	1.52	0.74
35:BD:247:MET:HG2	35:BD:248:SER:O	1.86	0.74
50:BU:67:ARG:HD3	50:BU:89:ARG:CZ	2.17	0.74
29:B5:33:LYS:NZ	33:BA:2373:U:OP1	2.19	0.74
33:BA:1829:C:H42	33:BA:1846:G:H22	1.33	0.74
33:BA:1364:C:C2	51:BV:86:ARG:NH2	2.55	0.74
52:BW:32:VAL:O	52:BW:77:ARG:NH1	2.21	0.74
34:BB:76:A:H62	34:BB:96:G:H21	1.35	0.74
35:BD:243:ARG:HH22	35:BD:247:MET:HB3	1.51	0.74
37:BF:67:GLN:HE22	37:BF:74:ARG:CB	2.01	0.74
47:BR:65:VAL:HG13	47:BR:73:ALA:HB1	1.70	0.73
50:BU:68:ALA:N	50:BU:90:GLN:O	2.20	0.73
43:BN:24:VAL:HG12	43:BN:26:GLY:H	1.53	0.73
33:BA:1353:C:N3	33:BA:1377:G:N2	2.35	0.73
33:BA:2039:G:H5"	51:BV:42:ALA:HB2	1.71	0.73
33:BA:2295:A:H62	33:BA:2302:A:H62	1.35	0.73
37:BF:66:ARG:NH1	37:BF:70:THR:CG2	2.47	0.73
22:AY:8:G:C6	22:AY:9:A:C6	2.77	0.73
22:AY:10:U:O2'	22:AY:11:G:OP1	2.07	0.73
33:BA:785:C:N4	33:BA:805:G:H1	1.86	0.72
1:AA:850:U:H3	1:AA:855:G:H22	1.34	0.72
43:BN:88:ARG:HD3	43:BN:94:ARG:HH21	1.53	0.72
24:B0:44:PRO:HB2	24:B0:45:LYS:HG2	1.70	0.72
33:BA:1799:G:H1	33:BA:2011:U:H3	1.37	0.72
50:BU:25:LEU:HD12	50:BU:27:ALA:H	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AY:8:G:H3'	22:AY:9:A:H8	1.55	0.72
33:BA:1474:C:H42	33:BA:1618:A:H62	1.37	0.72
50:BU:8:GLY:HA3	50:BU:10:LYS:H	1.53	0.72
33:BA:2552:G:H1	33:BA:2569:C:H42	1.37	0.72
53:BX:86:GLU:O	53:BX:87:ASP:CB	2.38	0.72
50:BU:67:ARG:HD3	50:BU:89:ARG:NH1	2.04	0.72
33:BA:2031:G:OP1	46:BQ:13:ARG:NH2	2.23	0.71
1:AA:861:U:O4	1:AA:862:A:N6	2.23	0.71
44:BO:23:ILE:CG2	50:BU:81:ASN:O	2.37	0.71
36:BE:123:ILE:HD13	36:BE:141:ARG:HE	1.55	0.71
35:BD:243:ARG:HH22	35:BD:247:MET:HB2	1.56	0.71
27:B3:51:SER:HA	27:B3:52:ALA:HB3	1.72	0.71
1:AA:965:U:N3	1:AA:1234:A:C2	2.58	0.71
33:BA:2123:A:H61	33:BA:2224:U:H3	1.35	0.71
22:AY:5:A:C5	22:AY:6:A:C8	2.79	0.71
21:AX:71:C:H5"	21:AX:71:C:H6	1.56	0.71
33:BA:1654:A:N6	33:BA:1692:U:O4	2.17	0.71
33:BA:875:U:H3	33:BA:876:A:H62	1.36	0.71
48:BS:63:THR:HG22	48:BS:76:THR:HG22	1.73	0.70
21:AX:72:C:C6	21:AX:72:C:H5"	2.25	0.70
33:BA:1317:G:O2'	46:BQ:27:ASN:ND2	2.24	0.70
33:BA:607:G:H21	49:BT:37:GLN:HE22	1.37	0.70
33:BA:1894:U:O2	33:BA:1905:A:N7	2.25	0.70
33:BA:957:A:H62	45:BP:12:GLU:HA	1.57	0.70
33:BA:1250:G:C5'	33:BA:1251:U:H5"	2.21	0.70
33:BA:831:U:H5	33:BA:840:A:C2	2.09	0.70
33:BA:1659:A:C2	51:BV:93:ALA:HB2	2.27	0.70
11:AK:38:ASP:O	11:AK:41:GLY:HA2	1.91	0.70
1:AA:970:U:H2'	1:AA:1234:A:H62	1.57	0.70
29:B5:2:ARG:HD2	29:B5:20:LYS:HB3	1.74	0.70
37:BF:154:ILE:HG12	37:BF:193:LEU:HD12	1.73	0.70
47:BR:65:VAL:HG13	47:BR:73:ALA:CB	2.21	0.69
33:BA:831:U:C5	33:BA:840:A:C2	2.80	0.69
1:AA:437:U:H3	1:AA:439:A:H62	1.37	0.69
33:BA:1347:A:H62	33:BA:1651:G:H8	1.38	0.69
33:BA:785:C:N3	33:BA:805:G:N2	2.38	0.69
42:BM:19:VAL:HG13	42:BM:143:LEU:HD11	1.72	0.69
33:BA:374:A:H2	33:BA:1250:G:H2'	1.53	0.69
24:B0:40:VAL:HG12	24:B0:41:ASN:N	2.07	0.69
29:B5:33:LYS:HB3	29:B5:44:LEU:HD23	1.75	0.69
50:BU:8:GLY:HA3	50:BU:10:LYS:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B6:31:LEU:HD23	30:B6:42:LEU:HD11	1.73	0.69
33:BA:1815:A:H5''	33:BA:2009:G:N2	2.08	0.69
51:BV:88:ARG:HB2	51:BV:92:ARG:HB2	1.73	0.69
22:AY:8:G:H3'	22:AY:9:A:C8	2.28	0.69
21:AX:22:G:N7	21:AX:46:G:N2	2.32	0.69
22:AY:5:A:H2'	22:AY:6:A:C5'	2.22	0.69
33:BA:715:A:H2'	33:BA:717:A:H62	1.57	0.69
51:BV:72:SER:OG	51:BV:106:VAL:CG1	2.41	0.69
1:AA:732:U:N3	22:AY:7:C:O2'	2.26	0.68
33:BA:2009:G:C4	33:BA:2011:U:C5	2.80	0.68
38:BG:57:LEU:HD23	38:BG:65:PRO:HB3	1.75	0.68
33:BA:1364:C:N3	51:BV:86:ARG:NH2	2.41	0.68
47:BR:65:VAL:HG11	47:BR:73:ALA:HB1	1.74	0.68
33:BA:2009:G:C5	33:BA:2011:U:C4	2.82	0.68
39:BH:103:LYS:HG2	39:BH:117:VAL:HG22	1.73	0.68
33:BA:2766:G:H1	33:BA:2796:C:H42	1.41	0.68
53:BX:39:ASN:HB3	53:BX:61:ALA:HB3	1.74	0.68
33:BA:2374:G:H5'	33:BA:2376:C:H5'	1.74	0.68
1:AA:128:A:N6	1:AA:193:G:O2'	2.26	0.68
22:AY:3:U:H2'	22:AY:4:G:H8	1.57	0.68
38:BG:135:GLN:HE22	38:BG:150:ARG:H	1.41	0.68
33:BA:2613:U:C3'	33:BA:2614:U:H5'	2.24	0.68
23:AZ:88:GLU:O	33:BA:2090:G:N2	2.27	0.68
54:BZ:46:TYR:HB3	54:BZ:67:LEU:HD12	1.76	0.68
35:BD:142:HIS:ND1	35:BD:193:GLY:O	2.27	0.68
22:AY:11:G:O2'	22:AY:12:A:OP2	2.11	0.68
33:BA:738:C:OP1	35:BD:217:ARG:NH2	2.23	0.68
33:BA:2669:G:H1	33:BA:2803:C:H42	1.42	0.68
28:B4:38:LEU:HD11	28:B4:41:ARG:HD2	1.74	0.67
33:BA:2709:C:H5'	36:BE:193:PRO:HA	1.76	0.67
1:AA:965:U:O4	1:AA:1234:A:N1	2.27	0.67
52:BW:5:ARG:HA	52:BW:46:ILE:HD11	1.75	0.67
24:B0:37:ARG:HD3	24:B0:45:LYS:HD3	1.75	0.67
37:BF:73:ALA:HB3	37:BF:75:GLN:CG	2.24	0.67
1:AA:1245:A:H4'	1:AA:1313:G:H4'	1.76	0.67
53:BX:86:GLU:O	53:BX:87:ASP:HB3	1.94	0.67
33:BA:795:G:H5'	33:BA:796:A:OP2	1.94	0.67
33:BA:1257:C:OP1	49:BT:15:LYS:NZ	2.27	0.67
32:B8:30:PRO:HB2	33:BA:2556:C:H5'	1.75	0.67
35:BD:171:TYR:HB2	35:BD:183:MET:HB3	1.77	0.67
33:BA:651:U:O2	33:BA:667:A:N7	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AY:1:U:C2'	22:AY:2:G:H1'	2.24	0.67
33:BA:797:A:N3	33:BA:797:A:H2'	2.10	0.67
33:BA:1111:U:O2	33:BA:1119:A:N7	2.28	0.67
50:BU:67:ARG:HA	50:BU:90:GLN:O	1.95	0.67
33:BA:1518:G:H3'	33:BA:1519:C:H5''	1.77	0.67
1:AA:1367:U:O2	1:AA:1372:A:N7	2.27	0.67
39:BH:21:ASP:HB3	39:BH:22:ASN:CB	2.21	0.67
33:BA:2090:G:OP1	37:BF:68:LYS:NZ	2.25	0.67
35:BD:29:PRO:HB3	35:BD:63:ARG:HE	1.58	0.67
33:BA:1042:A:H5'	49:BT:92:ARG:HE	1.59	0.66
33:BA:1371:G:N7	33:BA:1654:A:O2'	2.26	0.66
26:B2:5:GLU:HB2	26:B2:57:LYS:HB3	1.77	0.66
33:BA:918:U:H3	33:BA:953:G:H1	1.42	0.66
1:AA:666:U:H3	1:AA:758:A:H61	1.43	0.66
48:BS:67:ILE:HA	48:BS:72:GLY:HA2	1.76	0.66
31:B7:24:ARG:HD3	31:B7:50:VAL:HG22	1.78	0.66
32:B8:29:ASN:HB2	32:B8:32:HIS:HD2	1.61	0.66
38:BG:78:ARG:HB3	38:BG:79:LEU:HB2	1.78	0.66
39:BH:13:SER:HB3	39:BH:14:ASP:HA	1.78	0.66
24:B0:45:LYS:CE	24:B0:46:LYS:HE2	2.26	0.66
37:BF:4:VAL:HG12	37:BF:5:ALA:H	1.59	0.66
36:BE:178:LYS:HB2	36:BE:187:LEU:HD12	1.77	0.66
33:BA:1711:G:H1	33:BA:2023:C:N4	1.93	0.66
50:BU:79:LYS:C	50:BU:80:LYS:HG2	2.16	0.65
43:BN:22:ILE:HD12	43:BN:40:VAL:HG12	1.75	0.65
43:BN:11:ALA:HB2	43:BN:83:ALA:HB1	1.77	0.65
36:BE:28:ILE:HB	36:BE:186:LEU:HB2	1.77	0.65
33:BA:2571:A:H4'	33:BA:2572:G:H5'	1.78	0.65
31:B7:8:ARG:NH1	33:BA:247:A:OP2	2.29	0.65
33:BA:1522:U:O2	33:BA:1563:G:N2	2.30	0.65
1:AA:1313:G:H21	1:AA:1342:A:H62	1.44	0.65
33:BA:507:A:H62	33:BA:516:G:H21	1.43	0.65
21:AX:35:U:H6	21:AX:35:U:H5'	1.61	0.65
38:BG:64:LYS:HD2	38:BG:65:PRO:HD2	1.78	0.65
33:BA:2818:C:O2'	33:BA:2917:G:N2	2.29	0.65
33:BA:1268:G:OP2	49:BT:12:LYS:NZ	2.30	0.65
33:BA:1931:C:H5''	35:BD:241:ILE:HG21	1.77	0.65
51:BV:72:SER:OG	51:BV:106:VAL:HG12	1.96	0.65
33:BA:1783:C:N3	33:BA:2745:U:O2'	2.29	0.65
22:AY:12:A:H1'	22:AY:13:G:P	2.37	0.65
36:BE:201:THR:CG2	36:BE:203:LYS:HG3	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:2105:U:OP2	33:BA:2267:G:N2	2.28	0.65
47:BR:56:ALA:HB3	47:BR:81:VAL:HG22	1.78	0.65
37:BF:36:ALA:HB1	37:BF:183:VAL:HG21	1.79	0.65
1:AA:268:G:N2	1:AA:273:G:C5	2.65	0.65
28:B4:16:ARG:NH2	33:BA:1304:G:OP1	2.30	0.65
1:AA:992:U:H4'	1:AA:993:A:H5'	1.79	0.65
33:BA:729:G:O6	33:BA:841:A:N6	2.30	0.64
33:BA:1250:G:H4'	33:BA:1251:U:OP2	1.96	0.64
22:AY:5:A:C6	22:AY:6:A:C5	2.86	0.64
36:BE:125:ARG:NH1	36:BE:163:ARG:O	2.29	0.64
24:B0:44:PRO:HB2	24:B0:45:LYS:CG	2.27	0.64
37:BF:37:ILE:HG23	37:BF:184:LEU:HD21	1.79	0.64
33:BA:1808:U:OP2	33:BA:1813:A:N6	2.29	0.64
24:B0:39:LEU:N	24:B0:39:LEU:HD12	2.11	0.64
31:B7:57:ARG:NH2	33:BA:880:C:O2'	2.30	0.64
37:BF:66:ARG:HH11	37:BF:70:THR:HG23	1.60	0.64
29:B5:22:ASN:ND2	33:BA:2315:A:OP2	2.31	0.64
37:BF:67:GLN:NE2	37:BF:74:ARG:HG2	2.12	0.64
35:BD:39:LYS:NZ	35:BD:57:GLY:O	2.30	0.64
33:BA:831:U:C5	33:BA:840:A:N1	2.66	0.64
33:BA:1019:A:O2'	33:BA:1227:G:N2	2.31	0.64
24:B0:45:LYS:HB3	24:B0:46:LYS:HA	1.80	0.64
33:BA:377:G:H4'	33:BA:378:C:OP1	1.96	0.64
30:B6:37:LYS:NZ	33:BA:515:G:OP2	2.27	0.64
31:B7:13:ARG:NH1	44:BO:61:LEU:O	2.31	0.64
33:BA:1096:A:H3'	33:BA:1097:A:H8	1.62	0.64
35:BD:164:VAL:HG12	35:BD:166:GLY:H	1.63	0.64
22:AY:1:U:H2'	22:AY:2:G:O2'	1.98	0.63
29:B5:29:ARG:HG3	29:B5:47:GLU:HB3	1.80	0.63
33:BA:1847:U:H5''	35:BD:157:SER:HB3	1.79	0.63
33:BA:831:U:O4	33:BA:840:A:N1	2.30	0.63
33:BA:1056:A:OP1	49:BT:66:ASN:ND2	2.31	0.63
33:BA:2009:G:C6	33:BA:2011:U:O4	2.50	0.63
33:BA:837:U:H4'	33:BA:838:C:OP1	1.96	0.63
42:BM:54:HIS:HB3	42:BM:122:LYS:HB3	1.80	0.63
38:BG:100:LEU:HD23	38:BG:103:LEU:HD12	1.80	0.63
1:AA:446:G:N2	1:AA:505:G:N7	2.45	0.63
33:BA:2777:A:H5''	39:BH:4:VAL:HG21	1.81	0.63
50:BU:67:ARG:HD3	50:BU:89:ARG:NE	2.13	0.63
22:AY:12:A:H1'	22:AY:13:G:OP1	1.98	0.63
31:B7:31:HIS:ND1	33:BA:2421:A:OP1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:BR:65:VAL:N	47:BR:66:GLU:HA	2.13	0.63
33:BA:1263:G:C6	50:BU:70:LYS:NZ	2.66	0.63
41:BK:15:ALA:HB2	41:BK:46:THR:CG2	2.21	0.63
22:AY:11:G:O2'	22:AY:12:A:P	2.57	0.63
40:BJ:26:ILE:HG13	40:BJ:114:GLU:HB2	1.81	0.63
33:BA:1123:A:O2'	41:BK:93:ASN:ND2	2.32	0.63
33:BA:528:G:O2'	33:BA:552:G:N2	2.31	0.62
1:AA:591:C:OP2	1:AA:767:G:N1	2.26	0.62
40:BJ:11:VAL:HA	40:BJ:66:GLN:HE21	1.64	0.62
1:AA:1546:C:H2'	1:AA:1547:U:H6	1.64	0.62
51:BV:89:ALA:O	51:BV:92:ARG:HG2	1.99	0.62
51:BV:6:VAL:HG22	51:BV:104:THR:HG22	1.80	0.62
1:AA:458:G:O6	1:AA:493:G:O6	2.18	0.62
1:AA:1412:C:N4	22:AY:19:C:OP1	2.31	0.62
1:AA:1544:A:H8	1:AA:1544:A:O5'	1.81	0.62
33:BA:798:A:H5''	33:BA:799:A:OP1	1.98	0.62
51:BV:92:ARG:HA	51:BV:92:ARG:HE	1.64	0.62
1:AA:965:U:H3	1:AA:1234:A:H2	1.42	0.62
43:BN:16:ALA:HB2	43:BN:52:VAL:HG11	1.82	0.62
54:BZ:78:GLU:O	54:BZ:86:LYS:N	2.32	0.62
33:BA:839:G:H4'	33:BA:840:A:H5'	1.81	0.62
35:BD:132:LEU:HD23	35:BD:135:ILE:HD12	1.81	0.62
33:BA:1250:G:H4'	33:BA:1251:U:H5''	1.81	0.62
33:BA:2010:A:H3'	33:BA:2011:U:H5'	1.82	0.62
33:BA:793:U:H5'	33:BA:795:G:H1'	1.80	0.62
33:BA:1250:G:H5''	33:BA:1251:U:H5''	1.82	0.62
33:BA:1024:G:N2	33:BA:1031:C:N3	2.41	0.62
22:AY:10:U:H1'	22:AY:11:G:OP1	1.99	0.62
22:AY:10:U:O2'	22:AY:11:G:C5	2.49	0.62
33:BA:1846:G:OP1	35:BD:87:ARG:NH2	2.33	0.62
47:BR:113:ALA:HB1	47:BR:118:LEU:HD12	1.81	0.62
33:BA:1897:C:H42	33:BA:1902:G:H1	1.45	0.62
33:BA:835:A:H5''	33:BA:837:U:H5	1.65	0.62
33:BA:2128:U:H2'	33:BA:2129:G:H8	1.65	0.62
24:B0:43:LYS:O	24:B0:44:PRO:O	2.18	0.61
37:BF:65:TRP:HZ2	37:BF:75:GLN:HB2	1.51	0.61
45:BP:78:PRO:HG2	45:BP:81:VAL:HG21	1.82	0.61
42:BM:18:VAL:HG13	42:BM:58:ILE:HD13	1.82	0.61
33:BA:41:A:H2	33:BA:485:U:H3	1.47	0.61
33:BA:2434:G:H4'	44:BO:69:ILE:HD12	1.82	0.61
30:B6:1:MET:HG3	33:BA:800:G:OP1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AX:34:G:C2	21:AX:35:U:C6	2.88	0.61
33:BA:2730:U:O4	33:BA:2735:A:N1	2.33	0.61
31:B7:14:PHE:HB3	31:B7:22:LEU:HD23	1.82	0.61
33:BA:1291:A:OP1	49:BT:13:ARG:NH2	2.32	0.61
33:BA:2479:A:N6	33:BA:2530:C:O2	2.33	0.61
33:BA:678:A:H2'	33:BA:679:A:H8	1.65	0.61
22:AY:5:A:C2	22:AY:6:A:C1'	2.84	0.61
22:AY:10:U:H1'	22:AY:11:G:P	2.40	0.61
41:BK:15:ALA:CA	41:BK:46:THR:HG21	2.30	0.61
1:AA:1096:U:H3	1:AA:1109:G:H22	1.48	0.61
40:BJ:29:ASP:HB2	40:BJ:81:ALA:HB1	1.82	0.61
33:BA:1706:G:N2	33:BA:2717:G:OP1	2.34	0.61
33:BA:811:A:H5''	35:BD:209:GLY:HA2	1.83	0.61
33:BA:2518:G:N2	33:BA:2520:U:O4	2.33	0.61
33:BA:350:U:O2'	33:BA:1251:U:C5	2.52	0.61
33:BA:839:G:C4'	33:BA:840:A:H5'	2.31	0.61
40:BJ:28:VAL:HG12	40:BJ:30:TYR:H	1.65	0.61
39:BH:59:GLN:HB2	39:BH:62:HIS:HD2	1.66	0.61
31:B7:32:LEU:O	31:B7:36:LYS:NZ	2.33	0.61
33:BA:1065:U:N3	33:BA:1188:A:N6	2.48	0.61
33:BA:2900:A:HO2'	48:BS:5:GLN:N	1.98	0.61
45:BP:2:LEU:O	45:BP:44:ASN:ND2	2.33	0.60
31:B7:41:LYS:NZ	33:BA:2448:U:OP1	2.26	0.60
22:AY:5:A:C6	22:AY:6:A:C4	2.89	0.60
33:BA:1829:C:N4	33:BA:1846:G:H22	1.98	0.60
33:BA:1928:A:H4'	33:BA:1930:A:H5''	1.82	0.60
33:BA:797:A:N3	33:BA:799:A:H5'	2.16	0.60
37:BF:126:LEU:HD13	37:BF:193:LEU:HD22	1.82	0.60
33:BA:2613:U:H2'	33:BA:2614:U:H5'	1.84	0.60
33:BA:498:U:O2	33:BA:500:A:N6	2.34	0.60
33:BA:609:C:H5	50:BU:79:LYS:HE2	1.67	0.60
1:AA:965:U:N3	1:AA:1234:A:H2	1.98	0.60
32:B8:18:ARG:HA	32:B8:23:VAL:HA	1.82	0.60
33:BA:644:G:H1	33:BA:704:U:H3	1.50	0.60
1:AA:69:C:H2'	1:AA:70:G:C8	2.36	0.60
51:BV:6:VAL:HG12	51:BV:8:ARG:HG3	1.82	0.60
30:B6:34:ARG:CG	30:B6:42:LEU:HD12	2.14	0.60
48:BS:30:ARG:HD3	48:BS:45:ILE:HD11	1.83	0.60
22:AY:7:C:H2'	22:AY:7:C:O2	2.00	0.60
33:BA:1815:A:H5''	33:BA:2009:G:H22	1.66	0.60
44:BO:75:ALA:HB1	44:BO:76:VAL:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:636:G:H1	33:BA:712:C:H42	1.48	0.60
1:AA:385:G:O6	1:AA:386:A:N6	2.35	0.60
33:BA:787:C:H42	33:BA:804:G:H1	1.49	0.60
33:BA:1537:G:H2'	33:BA:1538:G:H8	1.67	0.60
1:AA:673:G:H22	1:AA:750:G:H1	1.50	0.60
33:BA:1835:C:O2	35:BD:44:ASN:ND2	2.35	0.60
24:B0:43:LYS:HB3	24:B0:44:PRO:HD2	1.83	0.59
24:B0:29:TRP:HZ3	33:BA:426:G:H21	1.50	0.59
33:BA:41:A:N1	33:BA:485:U:O4	2.35	0.59
33:BA:1250:G:H4'	33:BA:1251:U:C5'	2.32	0.59
37:BF:66:ARG:HD3	37:BF:70:THR:HG23	1.83	0.59
42:BM:57:ILE:HD12	42:BM:125:VAL:HG22	1.82	0.59
33:BA:1501:U:O4	33:BA:2733:C:N3	2.35	0.59
33:BA:2123:A:N6	33:BA:2224:U:H3	2.00	0.59
33:BA:830:A:H2'	33:BA:831:U:H4'	1.84	0.59
31:B7:27:ALA:HB3	33:BA:2390:A:H5'	1.82	0.59
1:AA:1549:C:C2	1:AA:1550:U:C6	2.91	0.59
33:BA:902:G:O2'	54:BZ:35:ASP:OD2	2.20	0.59
33:BA:822:G:H4'	33:BA:823:G:H5'	1.84	0.59
33:BA:576:G:N2	33:BA:2052:A:OP2	2.34	0.59
37:BF:73:ALA:CB	37:BF:75:GLN:HG2	2.27	0.59
35:BD:241:ILE:O	35:BD:241:ILE:HG23	2.01	0.59
42:BM:65:LEU:HD13	42:BM:69:LYS:HB2	1.85	0.59
33:BA:2855:G:OP1	36:BE:78:ARG:NH2	2.35	0.59
33:BA:2833:U:H2'	33:BA:2834:A:H8	1.66	0.59
33:BA:106:G:H2'	33:BA:107:G:H8	1.68	0.59
33:BA:515:G:O2'	37:BF:62:ARG:NH2	2.36	0.59
33:BA:1834:C:N4	33:BA:1841:G:H1	1.98	0.59
33:BA:721:G:H5''	37:BF:76:GLY:H	1.67	0.59
1:AA:1551:U:H3	22:AY:2:G:N2	1.91	0.59
44:BO:117:LEU:HB2	44:BO:119:LYS:N	2.17	0.59
1:AA:412:G:N2	1:AA:507:A:O2'	2.36	0.59
33:BA:1173:A:O2'	33:BA:1174:A:H5''	2.01	0.59
33:BA:2487:U:H2'	33:BA:2487:U:O2	2.02	0.59
35:BD:15:GLY:O	35:BD:204:ASN:ND2	2.35	0.59
53:BX:16:ASP:HB3	53:BX:19:LYS:HD2	1.85	0.59
33:BA:217:G:N1	33:BA:218:G:C6	2.71	0.59
21:AX:36:C:H5''	21:AX:36:C:H6	1.68	0.59
33:BA:1394:G:OP1	35:BD:43:ARG:NH2	2.35	0.59
22:AY:12:A:O2'	22:AY:13:G:OP1	2.15	0.59
33:BA:2785:U:O2'	33:BA:2786:A:OP2	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BV:92:ARG:NE	51:BV:92:ARG:HA	2.18	0.58
53:BX:86:GLU:HG3	53:BX:87:ASP:H	1.68	0.58
50:BU:10:LYS:HG3	50:BU:12:ILE:HD11	1.85	0.58
33:BA:1245:G:OP2	33:BA:1245:G:N2	2.34	0.58
33:BA:673:A:O2'	33:BA:674:G:O4'	2.21	0.58
33:BA:264:G:O2'	33:BA:654:G:O2'	2.20	0.58
39:BH:88:LEU:HB2	39:BH:132:VAL:HB	1.84	0.58
33:BA:1578:G:N2	33:BA:1587:U:OP2	2.36	0.58
33:BA:1207:C:H1'	50:BU:9:GLY:H	1.68	0.58
33:BA:861:C:O2'	33:BA:1264:G:N2	2.36	0.58
33:BA:588:C:N4	33:BA:589:G:O6	2.36	0.58
33:BA:350:U:H4'	33:BA:1251:U:H5	1.67	0.58
33:BA:2613:U:C2'	33:BA:2614:U:H5'	2.33	0.58
33:BA:1101:G:H4'	40:BJ:33:LEU:HA	1.85	0.58
1:AA:1295:C:H2'	1:AA:1296:A:H4'	1.84	0.58
37:BF:67:GLN:HE22	37:BF:74:ARG:CG	2.16	0.58
33:BA:1365:U:HO2'	33:BA:2039:G:HO2'	1.51	0.58
26:B2:7:THR:HG22	26:B2:34:THR:HG22	1.86	0.58
52:BW:20:LEU:HD22	52:BW:25:LYS:HD2	1.85	0.58
33:BA:377:G:C4	33:BA:378:C:C5	2.92	0.58
1:AA:1323:C:N4	1:AA:1332:G:H1	1.99	0.58
24:B0:45:LYS:NZ	24:B0:46:LYS:HE2	2.19	0.58
26:B2:5:GLU:HG2	26:B2:36:VAL:HG22	1.86	0.58
33:BA:673:A:H62	44:BO:78:ASN:ND2	2.02	0.58
33:BA:792:G:H5'	33:BA:793:U:OP2	2.04	0.58
33:BA:2717:G:N1	33:BA:2749:U:OP2	2.36	0.58
35:BD:150:LYS:HG2	35:BD:153:GLN:HE22	1.68	0.58
33:BA:934:U:H4'	33:BA:935:A:H8	1.69	0.58
33:BA:1261:C:N3	33:BA:1268:G:O6	2.36	0.57
33:BA:835:A:H5''	33:BA:837:U:C5	2.39	0.57
33:BA:2714:G:OP2	48:BS:52:LYS:NZ	2.37	0.57
33:BA:683:A:O2'	33:BA:684:G:OP2	2.22	0.57
34:BB:112:C:H2'	34:BB:113:A:H8	1.69	0.57
24:B0:3:ARG:NH1	33:BA:1403:G:OP1	2.36	0.57
36:BE:177:VAL:HG12	36:BE:178:LYS:HG3	1.86	0.57
31:B7:38:GLN:HA	31:B7:41:LYS:HD3	1.86	0.57
38:BG:47:ALA:N	38:BG:48:LYS:HA	2.19	0.57
33:BA:2799:C:C5	33:BA:2800:C:C6	2.93	0.57
33:BA:831:U:C4	33:BA:840:A:N1	2.72	0.57
35:BD:214:LYS:N	35:BD:215:GLY:HA2	2.19	0.57
30:B6:21:ARG:NH2	33:BA:513:A:OP1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BH:39:HIS:CE1	39:BH:42:MET:HG2	2.40	0.57
33:BA:2472:C:H2'	33:BA:2473:G:H8	1.69	0.57
1:AA:1154:C:H4'	1:AA:1155:A:O5'	2.04	0.57
37:BF:136:THR:HG22	37:BF:167:ALA:H	1.69	0.57
33:BA:1897:C:N4	33:BA:1902:G:H1	2.03	0.57
38:BG:40:VAL:HG12	38:BG:42:ASP:H	1.68	0.57
33:BA:881:U:O4	33:BA:882:A:N6	2.38	0.57
52:BW:47:PHE:HD1	52:BW:90:ILE:HD13	1.70	0.57
45:BP:137:ILE:N	45:BP:138:GLY:HA3	2.19	0.57
47:BR:91:SER:OG	47:BR:92:ASP:N	2.36	0.57
40:BJ:27:ILE:HB	40:BJ:83:ALA:HB3	1.86	0.57
33:BA:1855:C:O2'	33:BA:2000:A:OP2	2.22	0.57
33:BA:794:U:C4	33:BA:2642:U:C5	2.93	0.57
44:BO:55:MET:O	44:BO:60:ARG:NH1	2.38	0.57
33:BA:910:A:O2'	34:BB:98:G:O2'	2.21	0.57
36:BE:185:LEU:HD21	48:BS:7:LEU:HD21	1.86	0.57
33:BA:2071:A:N6	42:BM:117:ARG:HH12	2.03	0.57
24:B0:37:ARG:CG	24:B0:45:LYS:CG	2.76	0.57
33:BA:1829:C:N3	33:BA:1846:G:N1	2.43	0.57
33:BA:837:U:H3'	33:BA:837:U:H6	1.70	0.57
21:AX:36:C:N4	21:AX:37:A:N6	2.52	0.57
41:BK:46:THR:HG22	41:BK:46:THR:O	2.05	0.57
44:BO:117:LEU:HB2	44:BO:119:LYS:H	1.69	0.57
27:B3:48:LYS:O	27:B3:50:ALA:N	2.37	0.57
1:AA:106:G:H5'	1:AA:107:A:H5''	1.87	0.57
7:AG:18:TYR:O	7:AG:20:SER:N	2.34	0.57
33:BA:1828:G:O2'	35:BD:182:ARG:NH2	2.38	0.56
33:BA:2423:C:H5''	44:BO:63:LYS:HE3	1.87	0.56
33:BA:1600:G:O2'	33:BA:1601:A:O4'	2.22	0.56
49:BT:95:LEU:HD12	49:BT:98:LEU:HD11	1.85	0.56
1:AA:1293:C:H3'	1:AA:1294:A:H8	1.69	0.56
33:BA:1108:G:H2'	33:BA:1109:G:H8	1.70	0.56
26:B2:6:ILE:HG23	26:B2:54:VAL:HG13	1.88	0.56
43:BN:70:ARG:HG3	43:BN:76:TYR:HE1	1.70	0.56
33:BA:2154:G:H21	33:BA:2202:A:H62	1.53	0.56
48:BS:95:VAL:HG12	48:BS:97:ARG:H	1.69	0.56
44:BO:78:ASN:HB2	44:BO:81:LYS:HG2	1.85	0.56
42:BM:17:LEU:HB2	42:BM:55:VAL:HG22	1.87	0.56
41:BK:85:ILE:HD12	41:BK:98:ALA:HB2	1.88	0.56
1:AA:1087:G:N2	1:AA:1090:A:OP2	2.38	0.56
42:BM:42:LYS:NZ	42:BM:51:THR:O	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1110:C:N4	1:AA:1113:C:OP1	2.39	0.56
38:BG:24:SER:O	38:BG:26:MET:N	2.33	0.56
33:BA:2489:U:H5	33:BA:2521:U:H3	1.53	0.56
51:BV:21:MET:HA	51:BV:24:ILE:HD12	1.87	0.56
22:AY:12:A:C1'	22:AY:13:G:P	2.94	0.56
33:BA:839:G:H4'	33:BA:840:A:N3	2.20	0.56
33:BA:2267:G:H1'	33:BA:2269:C:H5	1.69	0.56
31:B7:32:LEU:HD11	31:B7:35:ASN:HD22	1.71	0.56
33:BA:787:C:H2'	33:BA:788:G:H5''	1.88	0.56
33:BA:1528:U:H4'	33:BA:1529:G:H5'	1.88	0.56
24:B0:45:LYS:HE3	24:B0:46:LYS:CE	2.35	0.56
33:BA:854:U:H2'	33:BA:855:G:C8	2.40	0.56
47:BR:65:VAL:CG1	47:BR:73:ALA:HB2	2.35	0.56
39:BH:12:PRO:O	39:BH:13:SER:HB2	2.06	0.56
33:BA:934:U:O2'	33:BA:935:A:O5'	2.23	0.56
40:BJ:53:LYS:HB3	40:BJ:55:TYR:HD2	1.70	0.56
1:AA:1544:A:C5'	1:AA:1544:A:C8	2.89	0.56
21:AX:56:C:O2'	21:AX:57:G:O4'	2.23	0.56
50:BU:14:VAL:HG11	50:BU:97:ILE:HD12	1.87	0.56
37:BF:65:TRP:HZ2	37:BF:75:GLN:CG	2.19	0.55
33:BA:805:G:HO2'	33:BA:2010:A:H8	1.55	0.55
33:BA:426:G:H1	33:BA:442:C:N4	2.02	0.55
37:BF:63:LYS:HA	37:BF:76:GLY:O	2.06	0.55
36:BE:119:PHE:HA	36:BE:163:ARG:HA	1.87	0.55
35:BD:44:ASN:HB2	35:BD:50:THR:HG23	1.88	0.55
24:B0:17:ASN:HD21	24:B0:27:ARG:HD2	1.71	0.55
1:AA:64:U:O2'	1:AA:387:C:O2	2.23	0.55
21:AX:34:G:H2'	21:AX:35:U:H5''	1.88	0.55
47:BR:25:THR:HG21	47:BR:47:ASP:HB2	1.87	0.55
33:BA:921:G:OP1	45:BP:63:LYS:NZ	2.40	0.55
1:AA:1071:G:OP2	3:AC:2:GLY:N	2.39	0.55
33:BA:2535:U:H2'	33:BA:2535:U:O2	2.07	0.55
41:BK:55:PRO:HG2	41:BK:71:LYS:HB2	1.88	0.55
30:B6:31:LEU:HD22	30:B6:42:LEU:HD11	1.87	0.55
1:AA:113:G:H4'	1:AA:114:A:O5'	2.03	0.55
33:BA:1314:A:N6	33:BA:1335:A:H4'	2.21	0.55
47:BR:22:LEU:CD2	47:BR:94:VAL:CG1	2.78	0.55
33:BA:1067:A:H2'	33:BA:1068:G:H4'	1.88	0.55
51:BV:84:ARG:HB2	51:BV:96:ILE:HB	1.87	0.55
33:BA:827:G:N1	35:BD:229:ASP:OD2	2.35	0.55
53:BX:33:VAL:N	53:BX:63:ILE:O	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:2696:C:H1'	39:BH:110:TYR:HD1	1.71	0.55
42:BM:38:ARG:HH12	42:BM:111:PRO:HG3	1.71	0.55
34:BB:10:G:N1	54:BZ:79:ARG:O	2.40	0.55
54:BZ:80:PHE:N	54:BZ:84:ARG:O	2.39	0.55
33:BA:2147:U:N3	33:BA:2176:A:O2'	2.37	0.55
33:BA:673:A:H62	44:BO:78:ASN:HD22	1.54	0.55
45:BP:30:GLY:HA2	45:BP:107:SER:HB3	1.87	0.55
31:B7:24:ARG:NH2	33:BA:2389:A:OP1	2.40	0.55
38:BG:78:ARG:HD2	38:BG:79:LEU:HD13	1.88	0.55
33:BA:1931:C:H5"	35:BD:241:ILE:CG2	2.36	0.55
35:BD:140:VAL:HG11	35:BD:194:GLN:HB3	1.89	0.55
22:AY:3:U:OP2	22:AY:3:U:H5	1.90	0.55
35:BD:243:ARG:HH12	35:BD:247:MET:HE1	1.72	0.55
33:BA:1103:A:O2'	33:BA:1104:U:OP1	2.23	0.55
42:BM:131:HIS:HD2	42:BM:133:HIS:HB2	1.72	0.55
1:AA:799:A:OP1	21:AX:38:C:O2'	2.23	0.55
22:AY:1:U:H2'	22:AY:2:G:C1'	2.33	0.54
49:BT:103:LEU:HG	49:BT:104:THR:HG22	1.89	0.54
29:B5:21:LYS:HE2	29:B5:30:VAL:HB	1.88	0.54
33:BA:1111:U:O2	33:BA:1119:A:C5	2.60	0.54
43:BN:38:VAL:HG22	43:BN:61:VAL:HG22	1.89	0.54
33:BA:565:U:O3'	51:BV:25:ARG:NH1	2.40	0.54
24:B0:42:GLY:CA	24:B0:43:LYS:HD3	2.38	0.54
1:AA:1549:C:C4	22:AY:5:A:N6	2.75	0.54
50:BU:67:ARG:NH1	50:BU:89:ARG:NH1	2.49	0.54
22:AY:8:G:C5	22:AY:9:A:C5	2.95	0.54
1:AA:986:G:O5'	1:AA:1367:U:O2'	2.24	0.54
1:AA:48:G:O2'	1:AA:373:U:O2	2.24	0.54
27:B3:9:PHE:HZ	38:BG:62:GLY:HA3	1.71	0.54
33:BA:796:A:H61	33:BA:800:G:N2	1.99	0.54
26:B2:10:ARG:HB3	26:B2:53:LEU:HD13	1.88	0.54
1:AA:970:U:H2'	1:AA:1234:A:N6	2.21	0.54
33:BA:2344:U:OP1	38:BG:33:LYS:NZ	2.39	0.54
33:BA:1094:A:H1'	33:BA:1158:G:H21	1.73	0.54
1:AA:1549:C:C4	1:AA:1550:U:C5	2.95	0.54
48:BS:95:VAL:HG13	48:BS:100:LEU:HD21	1.88	0.54
31:B7:25:SER:OG	44:BO:64:ARG:NH1	2.39	0.54
25:B1:54:LYS:NZ	33:BA:72:U:OP2	2.40	0.54
46:BQ:17:LEU:HD21	46:BQ:39:GLU:CD	2.28	0.54
24:B0:37:ARG:CZ	24:B0:44:PRO:HG3	2.26	0.54
24:B0:37:ARG:CB	24:B0:45:LYS:HD3	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AY:3:U:O5'	22:AY:3:U:H6	1.91	0.54
21:AX:7:G:O2'	21:AX:49:G:O5'	2.24	0.54
35:BD:21:PHE:HB3	35:BD:24:ILE:HD12	1.90	0.54
35:BD:230:HIS:ND1	35:BD:231:PRO:HD2	2.23	0.54
1:AA:348:U:OP2	43:BN:97:ARG:NH2	2.39	0.54
46:BQ:22:THR:HG22	46:BQ:66:ILE:HG23	1.89	0.54
46:BQ:4:ARG:HH12	46:BQ:38:LYS:HD2	1.73	0.54
33:BA:1500:U:OP1	46:BQ:81:GLN:NE2	2.40	0.54
42:BM:26:LEU:N	42:BM:27:GLY:HA3	2.23	0.54
37:BF:54:ARG:NH2	37:BF:77:SER:OG	2.40	0.54
33:BA:1024:G:N1	33:BA:1031:C:N4	2.42	0.54
33:BA:794:U:H6	33:BA:794:U:O5'	1.89	0.54
37:BF:29:ASN:HD22	37:BF:108:LEU:HD21	1.73	0.54
33:BA:1581:A:C6	33:BA:1584:U:O2	2.60	0.54
36:BE:35:VAL:HG13	36:BE:49:ILE:HG23	1.88	0.54
22:AY:5:A:C2'	22:AY:6:A:C5'	2.85	0.54
26:B2:5:GLU:OE2	26:B2:59:GLN:NE2	2.41	0.54
1:AA:526:G:N2	1:AA:539:G:OP1	2.39	0.54
35:BD:248:SER:OG	35:BD:250:TRP:O	2.25	0.54
1:AA:66:G:N2	1:AA:70:G:O6	2.30	0.54
17:AQ:33:HIS:O	17:AQ:37:GLY:N	2.40	0.54
1:AA:1325:G:N1	1:AA:1328:A:OP2	2.40	0.54
33:BA:2747:G:O2'	33:BA:2872:U:OP1	2.26	0.54
26:B2:20:ARG:NH2	33:BA:1016:U:OP1	2.41	0.54
33:BA:848:G:O4'	37:BF:54:ARG:NH1	2.41	0.53
33:BA:510:G:N2	33:BA:513:A:OP2	2.40	0.53
35:BD:230:HIS:CG	35:BD:231:PRO:HD2	2.43	0.53
33:BA:2552:G:H1	33:BA:2569:C:N4	2.06	0.53
54:BZ:18:THR:O	54:BZ:20:ASN:N	2.39	0.53
33:BA:517:A:OP1	37:BF:79:ARG:NH1	2.41	0.53
54:BZ:64:ASP:HB3	54:BZ:66:THR:HG23	1.90	0.53
33:BA:1322:G:N2	33:BA:1325:A:OP2	2.41	0.53
33:BA:2900:A:O2'	48:BS:5:GLN:N	2.41	0.53
40:BJ:22:SER:OG	40:BJ:87:GLU:OE1	2.26	0.53
33:BA:683:A:H4'	33:BA:684:G:O5'	2.07	0.53
33:BA:367:G:O2'	33:BA:368:G:OP2	2.22	0.53
33:BA:51:G:H21	33:BA:117:A:H62	1.55	0.53
33:BA:377:G:N3	33:BA:378:C:C5	2.77	0.53
33:BA:797:A:H2	33:BA:799:A:C5'	2.19	0.53
33:BA:1066:A:O2'	33:BA:1067:A:O5'	2.22	0.53
33:BA:1070:G:H3'	33:BA:1071:G:H5''	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BT:28:LYS:HA	49:BT:34:VAL:HG23	1.91	0.53
33:BA:557:U:O2'	33:BA:1255:G:N2	2.39	0.53
1:AA:105:G:OP1	1:AA:333:A:N6	2.38	0.53
33:BA:1055:A:OP1	42:BM:40:LYS:NZ	2.41	0.53
33:BA:2345:U:O2'	38:BG:125:ARG:NH1	2.32	0.53
24:B0:45:LYS:HB2	33:BA:2246:G:OP1	2.09	0.53
33:BA:2800:C:O2'	36:BE:172:GLN:NE2	2.38	0.53
33:BA:1829:C:H42	33:BA:1846:G:N2	2.02	0.53
22:AY:8:G:C6	22:AY:9:A:C5	2.97	0.53
40:BJ:58:THR:HG22	40:BJ:84:PHE:CD2	2.44	0.53
33:BA:1568:G:OP2	33:BA:1568:G:N2	2.34	0.53
45:BP:119:ARG:O	45:BP:122:SER:OG	2.22	0.53
33:BA:1127:U:OP1	41:BK:126:ARG:NH1	2.41	0.53
51:BV:89:ALA:O	51:BV:90:MET:CB	2.55	0.53
33:BA:1968:U:OP1	33:BA:2633:U:O2'	2.26	0.53
29:B5:34:LYS:HB2	29:B5:45:HIS:CE1	2.43	0.53
33:BA:1474:C:N4	33:BA:1618:A:H62	2.07	0.53
21:AX:55:U:H3'	21:AX:56:C:H5"	1.91	0.53
33:BA:1755:C:O2'	33:BA:1756:U:OP1	2.24	0.53
11:AK:37:THR:CA	11:AK:42:ASN:O	2.57	0.53
1:AA:518:A:H5'	4:AD:48:GLY:HA3	1.89	0.53
48:BS:78:PRO:HG2	48:BS:81:THR:HB	1.89	0.53
33:BA:2524:G:OP1	45:BP:82:ARG:NE	2.35	0.53
27:B3:6:HIS:HE1	38:BG:64:LYS:H	1.55	0.53
39:BH:4:VAL:O	39:BH:70:ARG:NE	2.42	0.53
33:BA:2479:A:N6	33:BA:2530:C:C2	2.77	0.53
1:AA:1074:G:O2'	1:AA:1199:G:N2	2.42	0.53
54:BZ:73:GLY:HA2	54:BZ:92:VAL:HG23	1.90	0.53
49:BT:92:ARG:N	50:BU:11:GLN:OE1	2.42	0.53
1:AA:1365:G:H2'	1:AA:1366:A:C8	2.44	0.53
34:BB:11:A:H8	34:BB:67:G:H21	1.54	0.53
25:B1:8:ASP:HB3	25:B1:13:GLU:HG3	1.91	0.53
22:AY:2:G:N3	22:AY:2:G:C2'	2.64	0.53
41:BK:19:ASN:H	41:BK:20:PRO:HD2	1.72	0.53
33:BA:2871:G:OP1	48:BS:55:GLY:N	2.41	0.53
35:BD:182:ARG:HG3	35:BD:269:PHE:HB3	1.91	0.52
53:BX:48:THR:HB	53:BX:49:GLN:C	2.30	0.52
24:B0:25:SER:HG	33:BA:2109:G:HO2'	1.54	0.52
33:BA:2351:A:O2'	33:BA:2352:G:OP1	2.25	0.52
1:AA:692:G:H1	1:AA:716:U:H3	1.56	0.52
50:BU:90:GLN:OE1	50:BU:91:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BF:186:VAL:HG13	37:BF:192:LEU:HD21	1.91	0.52
33:BA:1524:A:H2'	33:BA:1525:G:C8	2.44	0.52
2:AB:35:ARG:O	2:AB:37:GLY:N	2.42	0.52
35:BD:145:GLU:HB2	35:BD:188:CYS:SG	2.49	0.52
22:AY:10:U:H6	22:AY:10:U:OP2	1.93	0.52
46:BQ:17:LEU:HD21	46:BQ:39:GLU:OE2	2.10	0.52
41:BK:10:LYS:HE2	41:BK:57:GLU:HG2	1.91	0.52
30:B6:34:ARG:HG3	30:B6:42:LEU:HD13	1.91	0.52
37:BF:62:ARG:O	37:BF:78:ILE:CD1	2.58	0.52
37:BF:67:GLN:NE2	37:BF:74:ARG:CG	2.71	0.52
22:AY:8:G:C3'	22:AY:9:A:H8	2.21	0.52
36:BE:201:THR:HG22	36:BE:203:LYS:HG3	1.91	0.52
37:BF:153:LEU:HB2	37:BF:192:LEU:HB2	1.92	0.52
41:BK:99:THR:HG22	41:BK:138:VAL:HB	1.90	0.52
33:BA:2324:C:H41	47:BR:17:ARG:HH12	1.58	0.52
37:BF:80:SER:CB	37:BF:83:TRP:HD1	2.10	0.52
51:BV:88:ARG:CB	51:BV:92:ARG:HB2	2.39	0.52
1:AA:495:U:H2'	1:AA:496:A:H8	1.74	0.52
21:AX:17:U:OP1	21:AX:60:U:O2'	2.22	0.52
24:B0:5:CYS:HG	24:B0:50:SER:HG	1.57	0.52
33:BA:1130:A:H4'	40:BJ:55:TYR:HA	1.91	0.52
1:AA:343:C:H2'	1:AA:344:A:C8	2.45	0.52
33:BA:1710:A:O2'	43:BN:1:MET:O	2.25	0.52
33:BA:2187:A:O2'	33:BA:2188:G:O4'	2.28	0.52
33:BA:1093:G:H21	33:BA:1157:A:H62	1.57	0.52
33:BA:2160:U:H5'	33:BA:2161:G:H5''	1.92	0.52
1:AA:1335:U:H2'	1:AA:1336:G:H8	1.74	0.52
34:BB:38:U:O2'	34:BB:39:A:OP1	2.27	0.52
33:BA:1039:G:OP1	49:BT:50:ARG:NH2	2.42	0.52
37:BF:151:LYS:HG2	37:BF:172:GLY:HA2	1.89	0.52
27:B3:12:ALA:H	27:B3:25:GLY:HA2	1.75	0.52
1:AA:960:U:H3	1:AA:1240:G:H1	1.57	0.52
22:AY:5:A:N3	22:AY:6:A:C1'	2.72	0.52
22:AY:5:A:C5	22:AY:6:A:N7	2.78	0.52
33:BA:2008:C:H2'	33:BA:2009:G:H5''	1.92	0.52
33:BA:78:U:H3	33:BA:107:G:H1	1.56	0.52
36:BE:114:SER:HB3	36:BE:169:ILE:HD12	1.92	0.52
1:AA:842:U:O2'	1:AA:843:U:OP1	2.26	0.52
1:AA:98:U:O2'	1:AA:99:A:OP1	2.24	0.52
50:BU:89:ARG:O	50:BU:89:ARG:HG3	2.10	0.52
18:AR:16:CYS:H	18:AR:51:GLY:HA3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:617:G:N1	33:BA:2060:A:OP1	2.35	0.52
1:AA:1545:C:H2'	1:AA:1545:C:O2	2.09	0.52
33:BA:1133:G:H1	33:BA:1148:C:H42	1.58	0.52
1:AA:778:G:H4'	1:AA:1523:A:H4'	1.92	0.52
49:BT:91:ASN:HD22	49:BT:109:LEU:HD21	1.75	0.52
33:BA:2816:C:H1'	36:BE:64:PRO:HB3	1.91	0.52
36:BE:8:ARG:NH1	36:BE:197:LYS:O	2.42	0.52
33:BA:732:A:H1'	33:BA:735:U:H3	1.74	0.52
34:BB:101:U:H2'	34:BB:102:A:H8	1.75	0.52
38:BG:29:PRO:HA	38:BG:159:THR:HB	1.92	0.52
22:AY:10:U:C1'	22:AY:11:G:P	2.98	0.51
36:BE:11:GLY:HA3	48:BS:8:ILE:HD11	1.92	0.51
33:BA:644:G:N2	33:BA:650:U:OP1	2.43	0.51
33:BA:1013:U:O4	33:BA:1014:A:N6	2.43	0.51
33:BA:573:C:OP2	33:BA:2808:U:N3	2.37	0.51
1:AA:1549:C:N3	1:AA:1550:U:C5	2.78	0.51
33:BA:831:U:C5	33:BA:840:A:H2	2.27	0.51
33:BA:1887:G:N2	33:BA:1912:G:O2'	2.40	0.51
45:BP:39:ALA:HB2	45:BP:99:PRO:HD3	1.91	0.51
43:BN:91:LYS:HE2	43:BN:111:PHE:CE1	2.45	0.51
33:BA:1873:U:H5"	35:BD:258:LYS:HG2	1.93	0.51
53:BX:82:GLY:N	53:BX:93:VAL:O	2.37	0.51
1:AA:400:G:HO2'	1:AA:492:C:HO2'	1.56	0.51
27:B3:14:VAL:HB	27:B3:22:PHE:HB2	1.92	0.51
33:BA:1202:A:O4'	49:BT:51:ARG:NH1	2.43	0.51
22:AY:11:G:HO2'	22:AY:12:A:P	2.33	0.51
21:AX:35:U:C6	21:AX:35:U:H5'	2.45	0.51
33:BA:854:U:H5'	33:BA:2474:G:H4'	1.91	0.51
38:BG:41:GLY:O	38:BG:43:ALA:N	2.43	0.51
33:BA:430:C:O2	33:BA:438:A:N6	2.43	0.51
33:BA:998:G:H21	33:BA:2296:A:H2	1.57	0.51
41:BK:24:VAL:HG13	41:BK:28:LEU:HD12	1.93	0.51
33:BA:89:U:H3'	33:BA:90:A:H8	1.75	0.51
51:BV:75:PHE:O	51:BV:104:THR:OG1	2.24	0.51
1:AA:901:U:H2'	1:AA:902:A:H8	1.74	0.51
1:AA:1274:C:H2'	1:AA:1275:G:H8	1.74	0.51
46:BQ:21:THR:HG22	46:BQ:44:VAL:HG22	1.91	0.51
33:BA:343:A:C2	33:BA:377:G:O2'	2.61	0.51
49:BT:92:ARG:HG3	49:BT:94:MET:HG2	1.91	0.51
33:BA:2071:A:H62	42:BM:117:ARG:HH12	1.59	0.51
35:BD:78:VAL:HG22	35:BD:94:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:527:A:O2'	53:BX:42:LYS:O	2.29	0.51
1:AA:988:A:O2'	1:AA:1330:U:O4	2.27	0.51
33:BA:2713:U:OP2	48:BS:54:ARG:NH1	2.42	0.51
33:BA:2140:U:OP2	33:BA:2174:C:N4	2.43	0.51
35:BD:124:ILE:HG23	35:BD:192:ILE:HD13	1.91	0.51
33:BA:2786:A:H3'	33:BA:2787:A:H5''	1.93	0.51
33:BA:199:A:H62	33:BA:878:G:H21	1.56	0.51
33:BA:1434:A:H4'	33:BA:1435:U:OP1	2.10	0.51
33:BA:275:A:H62	33:BA:296:G:H21	1.59	0.51
33:BA:2334:U:H3	38:BG:151:GLY:HA3	1.75	0.51
22:AY:5:A:C2'	22:AY:6:A:H5''	2.36	0.51
51:BV:86:ARG:HG2	51:BV:87:PRO:HD2	1.93	0.51
33:BA:2766:G:H1	33:BA:2796:C:N4	2.08	0.51
31:B7:24:ARG:HB2	44:BO:61:LEU:HD13	1.93	0.51
33:BA:1901:A:O2'	33:BA:1902:G:O5'	2.28	0.51
33:BA:106:G:H2'	33:BA:107:G:C8	2.46	0.51
33:BA:934:U:O2'	33:BA:936:C:OP2	2.23	0.51
33:BA:1527:C:O2'	33:BA:1528:U:OP1	2.27	0.51
33:BA:365:U:C6	37:BF:165:LEU:HD13	2.46	0.51
33:BA:2529:U:O2'	33:BA:2533:U:OP1	2.25	0.51
52:BW:59:TYR:HE2	52:BW:78:LYS:HE3	1.75	0.51
1:AA:1550:U:C2	22:AY:4:G:C2	2.98	0.51
33:BA:792:G:N2	33:BA:800:G:C6	2.79	0.51
53:BX:2:HIS:HD2	53:BX:81:VAL:HG21	1.76	0.51
43:BN:40:VAL:HG22	43:BN:59:LYS:HG2	1.91	0.51
33:BA:934:U:H4'	33:BA:935:A:C8	2.44	0.51
33:BA:1581:A:C5	33:BA:1584:U:O2	2.63	0.51
51:BV:40:PRO:O	51:BV:44:SER:OG	2.27	0.51
33:BA:793:U:H5'	33:BA:795:G:C1'	2.41	0.51
21:AX:72:C:H6	21:AX:72:C:C5'	2.17	0.51
35:BD:145:GLU:HA	35:BD:152:GLY:HA2	1.93	0.51
1:AA:154:C:H42	1:AA:165:G:H1	1.58	0.51
33:BA:1784:A:O2'	33:BA:1785:G:OP1	2.27	0.51
35:BD:53:HIS:HA	35:BD:217:ARG:HD2	1.93	0.50
1:AA:370:G:N2	1:AA:373:U:OP2	2.32	0.50
33:BA:2719:A:C2	46:BQ:17:LEU:CD1	2.93	0.50
42:BM:77:ARG:HH12	42:BM:88:ARG:HE	1.56	0.50
47:BR:79:GLU:HG2	47:BR:83:LYS:HE3	1.93	0.50
41:BK:8:VAL:HG22	41:BK:59:SER:HA	1.92	0.50
33:BA:2799:C:C5'	33:BA:2800:C:OP2	2.59	0.50
37:BF:62:ARG:O	37:BF:78:ILE:HD11	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:2785:U:C4	33:BA:2787:A:N7	2.79	0.50
1:AA:1153:G:H21	1:AA:1155:A:H62	1.57	0.50
33:BA:526:A:H1'	33:BA:527:A:H5''	1.93	0.50
33:BA:1629:C:N4	33:BA:1630:G:O6	2.45	0.50
31:B7:54:ASP:OD2	33:BA:2388:C:O2'	2.25	0.50
39:BH:104:LEU:HD22	39:BH:124:ILE:HG21	1.92	0.50
1:AA:683:G:H2'	1:AA:684:A:C8	2.46	0.50
33:BA:2794:A:OP2	33:BA:2795:G:N2	2.42	0.50
24:B0:43:LYS:C	24:B0:44:PRO:O	2.49	0.50
33:BA:1377:G:H5''	52:BW:14:THR:HG22	1.91	0.50
11:AK:38:ASP:C	11:AK:41:GLY:HA2	2.31	0.50
51:BV:41:ARG:HG3	51:BV:43:ALA:H	1.77	0.50
1:AA:1367:U:OP1	14:AN:35:ARG:N	2.43	0.50
33:BA:2876:A:O3'	46:BQ:60:ARG:NH1	2.45	0.50
1:AA:1314:G:H21	1:AA:1341:A:H2	1.59	0.50
26:B2:50:VAL:HG12	26:B2:53:LEU:HB3	1.92	0.50
39:BH:13:SER:CB	39:BH:14:ASP:HA	2.35	0.50
33:BA:338:G:H2'	33:BA:339:A:H8	1.76	0.50
33:BA:2785:U:O4	33:BA:2787:A:N7	2.45	0.50
33:BA:2815:U:OP1	36:BE:71:LYS:NZ	2.44	0.50
33:BA:248:G:OP2	44:BO:67:THR:OG1	2.24	0.50
33:BA:1631:A:H4'	33:BA:1632:G:H4'	1.93	0.50
1:AA:596:G:N2	1:AA:763:C:OP2	2.37	0.50
1:AA:317:G:H2'	1:AA:318:G:H8	1.76	0.50
33:BA:2738:G:H5''	46:BQ:18:ARG:HH22	1.76	0.50
33:BA:350:U:H4'	33:BA:1251:U:C5	2.45	0.50
33:BA:785:C:N4	33:BA:805:G:N1	2.49	0.50
33:BA:1365:U:O4	33:BA:1692:U:O2'	2.22	0.50
46:BQ:17:LEU:HD13	46:BQ:43:VAL:HG21	1.94	0.50
38:BG:29:PRO:HB2	38:BG:169:LEU:HD22	1.93	0.50
36:BE:126:HIS:CE1	36:BE:159:LEU:HD22	2.46	0.50
45:BP:36:ALA:HB2	45:BP:103:LEU:HD11	1.94	0.50
1:AA:1237:C:H2'	1:AA:1238:A:H8	1.76	0.50
33:BA:1174:A:N6	33:BA:2547:A:N6	2.60	0.50
1:AA:1058:G:H2'	1:AA:1060:G:H8	1.77	0.50
47:BR:32:ASN:HA	47:BR:96:ASP:HB2	1.92	0.50
29:B5:30:VAL:HG12	29:B5:47:GLU:HB2	1.94	0.50
35:BD:205:ILE:HG23	35:BD:210:ARG:HB2	1.94	0.50
33:BA:1432:A:O2'	33:BA:1433:U:H5'	2.12	0.50
53:BX:77:GLU:OE1	53:BX:96:LYS:NZ	2.39	0.50
39:BH:58:ASP:O	39:BH:63:ARG:NE	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:2488:A:OP2	33:BA:2489:U:OP2	2.30	0.50
40:BJ:27:ILE:O	40:BJ:83:ALA:N	2.45	0.50
45:BP:103:LEU:HD13	45:BP:125:LEU:HD13	1.94	0.50
33:BA:2629:A:O2'	33:BA:2630:C:H5'	2.12	0.50
33:BA:1339:A:H4'	33:BA:1340:A:O5'	2.11	0.50
1:AA:1265:C:O2'	1:AA:1287:C:N4	2.45	0.50
1:AA:62:A:N6	1:AA:108:C:N3	2.59	0.50
33:BA:1658:G:C2	33:BA:1664:G:C6	3.00	0.50
25:B1:40:THR:HA	25:B1:43:ILE:HD12	1.93	0.50
37:BF:53:ASN:OD1	37:BF:54:ARG:N	2.45	0.50
36:BE:16:PHE:O	48:BS:15:GLN:NE2	2.45	0.50
29:B5:7:LEU:HB2	29:B5:17:TYR:HB2	1.93	0.50
53:BX:49:GLN:N	53:BX:50:ALA:HA	2.27	0.49
1:AA:630:A:N6	1:AA:631:A:N6	2.60	0.49
33:BA:2382:G:N2	54:BZ:42:GLY:O	2.43	0.49
33:BA:2357:A:H2'	33:BA:2358:A:C8	2.47	0.49
37:BF:65:TRP:HZ2	37:BF:75:GLN:HG3	1.77	0.49
33:BA:721:G:H1'	37:BF:74:ARG:HD2	1.94	0.49
31:B7:9:GLY:O	31:B7:13:ARG:HG2	2.12	0.49
33:BA:997:C:H2'	33:BA:998:G:H8	1.77	0.49
36:BE:110:VAL:HG11	36:BE:192:VAL:HG13	1.92	0.49
33:BA:2009:G:H3'	33:BA:2010:A:H5''	1.93	0.49
1:AA:439:A:H2'	1:AA:440:A:H8	1.76	0.49
48:BS:55:GLY:HA2	48:BS:60:GLU:HG2	1.93	0.49
27:B3:56:VAL:HG11	27:B3:60:ASN:HD22	1.77	0.49
31:B7:21:LYS:HD2	31:B7:49:VAL:HG11	1.94	0.49
53:BX:10:MET:HG2	53:BX:71:LEU:HD11	1.93	0.49
39:BH:153:ARG:HG2	39:BH:162:GLY:HA3	1.93	0.49
33:BA:69:C:O2	33:BA:73:A:O2'	2.30	0.49
24:B0:45:LYS:HE3	24:B0:46:LYS:HE2	1.92	0.49
22:AY:1:U:C3'	22:AY:2:G:H1'	2.42	0.49
22:AY:1:U:O3'	22:AY:2:G:H4'	2.13	0.49
33:BA:364:A:O2'	33:BA:366:A:H2'	2.12	0.49
12:AL:26:LYS:N	12:AL:27:GLY:HA2	2.28	0.49
33:BA:648:G:O2'	33:BA:649:G:O5'	2.27	0.49
22:AY:6:A:H2'	22:AY:7:C:C6	2.47	0.49
24:B0:39:LEU:CD1	24:B0:39:LEU:N	2.76	0.49
33:BA:1659:A:N6	51:BV:88:ARG:O	2.44	0.49
28:B4:18:THR:HG22	33:BA:15:G:H4'	1.93	0.49
33:BA:568:G:O2'	33:BA:587:C:O2'	2.28	0.49
1:AA:95:U:H2'	1:AA:96:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BU:79:LYS:O	50:BU:80:LYS:HG2	2.13	0.49
33:BA:910:A:N6	33:BA:911:G:O6	2.46	0.49
52:BW:29:GLU:HA	52:BW:78:LYS:HA	1.94	0.49
33:BA:568:G:HO2'	33:BA:587:C:HO2'	1.60	0.49
46:BQ:31:GLU:HG2	46:BQ:116:ILE:HG12	1.94	0.49
33:BA:970:A:H2'	33:BA:971:A:C8	2.48	0.49
40:BJ:18:LYS:HA	40:BJ:21:GLU:HB2	1.95	0.49
46:BQ:106:PRO:HA	46:BQ:113:PRO:HA	1.95	0.49
35:BD:159:GLY:HA2	35:BD:198:GLU:HG2	1.94	0.49
33:BA:461:C:H2'	33:BA:462:A:C8	2.47	0.49
14:AN:47:LEU:O	14:AN:51:GLY:N	2.46	0.49
44:BO:117:LEU:HA	44:BO:118:GLU:CB	2.37	0.49
54:BZ:79:ARG:HG2	54:BZ:81:GLY:H	1.77	0.49
53:BX:48:THR:HA	53:BX:49:GLN:HB2	1.95	0.49
38:BG:39:GLY:O	38:BG:41:GLY:N	2.40	0.49
1:AA:616:A:OP1	1:AA:640:G:N2	2.37	0.49
33:BA:1929:A:H1'	33:BA:1999:A:H2'	1.94	0.49
47:BR:58:THR:HG22	47:BR:77:VAL:HG21	1.95	0.49
19:AS:81:LYS:H	19:AS:82:GLY:HA2	1.77	0.49
33:BA:1295:U:C5	37:BF:72:ARG:O	2.64	0.49
37:BF:65:TRP:CZ2	37:BF:75:GLN:HB3	2.43	0.49
1:AA:437:U:O2	1:AA:439:A:N7	2.45	0.49
40:BJ:26:ILE:HD13	40:BJ:116:LYS:HE3	1.94	0.49
42:BM:69:LYS:HA	42:BM:72:ASP:HB3	1.94	0.49
50:BU:73:VAL:N	50:BU:86:GLN:O	2.46	0.49
39:BH:96:ARG:HG3	39:BH:107:ASN:HD22	1.78	0.49
30:B6:34:ARG:NH2	33:BA:513:A:OP1	2.33	0.49
33:BA:565:U:H4'	51:BV:25:ARG:HH22	1.77	0.49
33:BA:2793:A:N6	33:BA:2795:G:N7	2.61	0.49
50:BU:73:VAL:HB	50:BU:86:GLN:O	2.12	0.49
33:BA:2728:U:H3	33:BA:2737:G:H1	1.59	0.49
33:BA:1452:C:H2'	33:BA:1453:A:H8	1.78	0.49
33:BA:2609:U:H5'	36:BE:137:SER:HA	1.94	0.49
1:AA:1385:U:H2'	1:AA:1386:A:H8	1.76	0.49
33:BA:2761:G:H5''	33:BA:2762:A:C8	2.47	0.49
35:BD:167:LYS:HB2	35:BD:172:VAL:HG22	1.95	0.49
33:BA:1250:G:C4'	33:BA:1251:U:H5''	2.42	0.49
1:AA:666:U:H3	1:AA:758:A:N6	2.10	0.49
44:BO:91:VAL:HG21	44:BO:121:LEU:HD22	1.94	0.49
33:BA:852:G:O4'	44:BO:38:GLN:NE2	2.46	0.49
33:BA:2342:C:H1'	38:BG:37:ASN:HD21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:2670:A:H5''	42:BM:79:THR:HG22	1.95	0.48
33:BA:2100:A:H2'	33:BA:2101:G:C8	2.48	0.48
48:BS:29:LEU:HB3	48:BS:89:VAL:HG22	1.95	0.48
35:BD:264:ASN:ND2	35:BD:266:SER:OG	2.46	0.48
33:BA:1398:A:N7	33:BA:1411:U:O4	2.46	0.48
42:BM:45:TYR:O	49:BT:64:ARG:NE	2.38	0.48
22:AY:13:G:H4'	22:AY:14:G:OP1	2.13	0.48
33:BA:2267:G:O2'	33:BA:2269:C:OP2	2.27	0.48
33:BA:588:C:N4	33:BA:589:G:C6	2.82	0.48
35:BD:108:LYS:HE3	35:BD:194:GLN:HE21	1.77	0.48
31:B7:60:GLN:NE2	33:BA:637:A:O2'	2.44	0.48
33:BA:2253:G:H4'	33:BA:2255:C:C2	2.48	0.48
33:BA:636:G:H1	33:BA:712:C:N4	2.10	0.48
33:BA:907:U:HO2'	33:BA:908:A:H8	1.59	0.48
49:BT:44:ASN:HB2	50:BU:76:TYR:CE2	2.47	0.48
33:BA:2605:G:O2'	33:BA:2608:C:OP2	2.30	0.48
22:AY:5:A:O2'	22:AY:6:A:O5'	2.23	0.48
33:BA:795:G:C5	33:BA:797:A:C5	3.01	0.48
29:B5:22:ASN:HD21	33:BA:2314:C:P	2.37	0.48
33:BA:1291:A:H5''	49:BT:13:ARG:NH2	2.29	0.48
33:BA:2856:G:OP1	36:BE:57:ARG:NH2	2.46	0.48
54:BZ:53:ILE:HG21	54:BZ:87:VAL:HG23	1.95	0.48
37:BF:64:PRO:HB2	37:BF:65:TRP:CE3	2.48	0.48
22:AY:8:G:C6	22:AY:9:A:N6	2.81	0.48
1:AA:1508:U:O2'	22:AY:18:A:OP1	2.17	0.48
33:BA:1524:A:H2'	33:BA:1525:G:H8	1.78	0.48
36:BE:139:TYR:HA	36:BE:142:ARG:HH21	1.79	0.48
25:B1:11:THR:HA	25:B1:14:ILE:HD12	1.95	0.48
23:AZ:81:ASN:N	23:AZ:81:ASN:ND2	2.60	0.48
33:BA:113:U:O2'	52:BW:33:ARG:NH1	2.46	0.48
24:B0:42:GLY:HA3	24:B0:43:LYS:HD3	1.95	0.48
33:BA:364:A:H4'	33:BA:366:A:H8	1.73	0.48
33:BA:1292:G:H1	49:BT:37:GLN:HE21	1.61	0.48
1:AA:126:G:O2'	1:AA:127:U:OP1	2.23	0.48
33:BA:52:A:H62	33:BA:118:A:H62	1.61	0.48
33:BA:1128:U:OP1	41:BK:119:ALA:N	2.43	0.48
33:BA:2082:G:H4'	36:BE:152:ASN:HD22	1.79	0.48
33:BA:1894:U:O2'	33:BA:1904:G:N2	2.45	0.48
33:BA:2572:G:H21	33:BA:2675:C:H5''	1.79	0.48
1:AA:766:U:H2'	1:AA:767:G:O4'	2.14	0.48
33:BA:1537:G:H2'	33:BA:1538:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B3:9:PHE:CZ	38:BG:62:GLY:HA3	2.49	0.48
33:BA:84:A:H3'	53:BX:4:LYS:HB2	1.95	0.48
33:BA:2683:A:O2'	33:BA:2684:G:O5'	2.25	0.48
1:AA:1227:C:H2'	1:AA:1228:U:C6	2.47	0.48
33:BA:1815:A:OP1	33:BA:2009:G:N2	2.45	0.48
35:BD:243:ARG:HH12	35:BD:247:MET:CE	2.26	0.48
33:BA:1364:C:C2	51:BV:86:ARG:NH1	2.82	0.48
1:AA:843:U:H2'	1:AA:844:A:C8	2.48	0.48
31:B7:20:GLY:HA2	31:B7:21:LYS:O	2.13	0.48
33:BA:83:G:H4'	33:BA:84:A:OP1	2.10	0.48
1:AA:23:G:H2'	1:AA:24:G:C8	2.48	0.48
49:BT:52:GLN:HA	49:BT:55:ARG:HG2	1.96	0.48
29:B5:15:ARG:NH2	33:BA:2427:U:O2'	2.35	0.48
41:BK:15:ALA:CB	41:BK:46:THR:HG22	2.05	0.48
33:BA:1353:C:N4	33:BA:1377:G:N1	2.43	0.48
28:B4:13:LYS:O	28:B4:17:ARG:HG2	2.14	0.48
33:BA:2784:C:O2'	33:BA:2785:U:O5'	2.24	0.48
46:BQ:78:ASP:HB3	46:BQ:81:GLN:HG3	1.96	0.48
33:BA:2576:U:HO2'	33:BA:2577:G:H8	1.62	0.48
36:BE:12:MET:SD	36:BE:26:THR:HG22	2.54	0.48
33:BA:681:C:O2'	33:BA:685:U:OP1	2.32	0.48
33:BA:972:U:HO2'	33:BA:973:G:H8	1.62	0.48
1:AA:732:U:C2	22:AY:7:C:O2'	2.67	0.48
22:AY:5:A:N1	22:AY:6:A:C4	2.82	0.48
33:BA:2039:G:OP2	51:BV:41:ARG:NH1	2.47	0.48
21:AX:34:G:C6	21:AX:35:U:C5	3.01	0.48
53:BX:48:THR:O	53:BX:52:PRO:HA	2.14	0.48
33:BA:1438:C:O2'	33:BA:1439:U:OP1	2.30	0.48
1:AA:547:U:H2'	1:AA:548:A:C8	2.49	0.48
1:AA:1117:C:OP1	3:AC:172:VAL:N	2.47	0.48
1:AA:1469:C:H2'	1:AA:1470:A:H8	1.79	0.48
47:BR:69:GLY:O	47:BR:105:ARG:NH2	2.47	0.48
33:BA:7:G:O6	33:BA:2919:A:N6	2.47	0.48
21:AX:23:A:H2'	21:AX:24:A:C8	2.48	0.48
24:B0:43:LYS:O	24:B0:44:PRO:C	2.50	0.47
1:AA:965:U:C4	1:AA:1234:A:N1	2.81	0.47
1:AA:956:A:H2'	1:AA:957:G:C8	2.49	0.47
37:BF:65:TRP:CH2	37:BF:72:ARG:NH2	2.83	0.47
33:BA:528:G:H2'	33:BA:553:A:H62	1.78	0.47
11:AK:39:THR:C	11:AK:41:GLY:HA2	2.35	0.47
48:BS:100:LEU:HB3	48:BS:103:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:852:G:H5'	33:BA:853:C:H5	1.79	0.47
1:AA:421:G:N2	1:AA:436:G:H1'	2.30	0.47
1:AA:404:A:O2'	1:AA:406:C:OP1	2.24	0.47
44:BO:20:GLY:HA2	44:BO:28:GLY:HA2	1.96	0.47
33:BA:377:G:N3	33:BA:378:C:C6	2.82	0.47
35:BD:53:HIS:HB2	35:BD:217:ARG:HB3	1.96	0.47
52:BW:9:LYS:HB2	52:BW:29:GLU:HB2	1.96	0.47
33:BA:2522:U:O2'	45:BP:80:GLU:OE2	2.23	0.47
33:BA:128:C:H5'	33:BA:1644:C:O2'	2.15	0.47
33:BA:1347:A:N6	33:BA:1651:G:H8	2.09	0.47
33:BA:2766:G:H2'	33:BA:2767:A:C8	2.50	0.47
33:BA:839:G:C4'	33:BA:840:A:C2	2.97	0.47
31:B7:57:ARG:NH2	44:BO:51:GLU:OE1	2.40	0.47
21:AX:37:A:C2	22:AY:17:G:C6	3.03	0.47
37:BF:20:ASN:ND2	37:BF:203:GLU:OE1	2.46	0.47
1:AA:987:A:N6	1:AA:1233:U:O5'	2.48	0.47
33:BA:1290:G:OP2	44:BO:21:ARG:NH1	2.47	0.47
21:AX:74:C:H5'	33:BA:2631:A:C5'	2.38	0.47
33:BA:875:U:H3	33:BA:876:A:N6	2.08	0.47
33:BA:2719:A:N1	46:BQ:39:GLU:OE2	2.47	0.47
33:BA:365:U:H3	33:BA:385:G:HO2'	1.57	0.47
33:BA:1658:G:C6	33:BA:1664:G:O6	2.68	0.47
33:BA:2386:U:OP1	54:BZ:28:ARG:NH1	2.48	0.47
33:BA:2853:C:H2'	33:BA:2854:A:H8	1.79	0.47
47:BR:71:THR:OG1	47:BR:72:SER:N	2.45	0.47
36:BE:176:ILE:HA	36:BE:188:ILE:HA	1.96	0.47
23:AZ:74:ILE:CA	51:BV:85:PHE:CD2	2.83	0.47
51:BV:92:ARG:HE	51:BV:92:ARG:CA	2.27	0.47
33:BA:874:U:H4'	33:BA:875:U:C6	2.50	0.47
1:AA:1313:G:N2	1:AA:1342:A:H62	2.10	0.47
33:BA:2815:U:O2'	36:BE:64:PRO:O	2.27	0.47
39:BH:3:ARG:HB2	39:BH:6:LYS:HE2	1.95	0.47
33:BA:1969:U:OP1	33:BA:2632:G:N2	2.42	0.47
36:BE:207:LYS:HA	36:BE:208:SER:HA	1.61	0.47
1:AA:643:C:H2'	1:AA:644:A:H8	1.80	0.47
45:BP:41:TRP:HB3	45:BP:94:VAL:HG11	1.97	0.47
30:B6:34:ARG:CB	30:B6:42:LEU:HD13	2.45	0.47
33:BA:1103:A:HO2'	33:BA:1104:U:P	2.37	0.47
1:AA:413:U:H1'	1:AA:507:A:H2'	1.97	0.47
35:BD:132:LEU:HA	35:BD:135:ILE:HD12	1.96	0.47
39:BH:158:TYR:HA	39:BH:173:LYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:694:G:H2'	33:BA:695:G:H8	1.79	0.47
3:AC:57:GLU:O	3:AC:64:ASN:N	2.44	0.47
1:AA:1501:G:O2'	1:AA:1502:A:OP1	2.29	0.47
37:BF:71:GLY:O	37:BF:72:ARG:HD2	2.15	0.47
24:B0:40:VAL:CG1	24:B0:41:ASN:H	2.13	0.47
22:AY:14:G:H2'	22:AY:15:A:C6	2.50	0.47
33:BA:2669:G:H1	33:BA:2803:C:N4	2.08	0.47
33:BA:2834:A:N6	33:BA:2835:A:N6	2.63	0.47
33:BA:1433:U:H2'	33:BA:1433:U:O2	2.14	0.47
1:AA:1525:C:H2'	1:AA:1526:G:C8	2.50	0.47
1:AA:954:G:N1	1:AA:1347:G:OP2	2.32	0.47
51:BV:3:ALA:HB2	51:BV:58:ALA:HB2	1.96	0.47
1:AA:1066:U:H2'	1:AA:1067:G:H8	1.79	0.47
1:AA:848:G:H2'	1:AA:849:G:C8	2.50	0.47
35:BD:170:LYS:HA	35:BD:171:TYR:HA	1.74	0.47
24:B0:14:ALA:HA	24:B0:28:THR:HA	1.97	0.47
53:BX:97:SER:HA	53:BX:98:GLY:HA2	1.64	0.47
33:BA:304:G:H2'	33:BA:305:A:H8	1.80	0.47
42:BM:46:THR:O	42:BM:49:VAL:HG12	2.15	0.47
1:AA:872:C:H1'	1:AA:884:G:H5'	1.96	0.47
30:B6:34:ARG:HB3	30:B6:42:LEU:HD13	1.98	0.46
33:BA:1656:C:O2'	33:BA:1657:C:C5'	2.58	0.46
33:BA:678:A:H2'	33:BA:679:A:C8	2.49	0.46
33:BA:822:G:H4'	33:BA:823:G:C5'	2.45	0.46
33:BA:567:U:H2'	33:BA:568:G:H8	1.80	0.46
37:BF:6:LEU:HD13	37:BF:7:TYR:N	2.30	0.46
33:BA:269:G:H1'	33:BA:322:A:H2	1.79	0.46
33:BA:1309:G:O2'	33:BA:1364:C:N4	2.47	0.46
37:BF:67:GLN:HE22	37:BF:74:ARG:HB3	1.78	0.46
42:BM:24:LYS:HE2	42:BM:143:LEU:HD22	1.97	0.46
31:B7:13:ARG:HD3	44:BO:63:LYS:HA	1.97	0.46
31:B7:57:ARG:HG3	31:B7:58:ILE:HG23	1.96	0.46
52:BW:20:LEU:HB3	52:BW:25:LYS:HG3	1.97	0.46
1:AA:1237:C:H2'	1:AA:1238:A:C8	2.50	0.46
1:AA:345:G:H2'	1:AA:346:A:C8	2.51	0.46
42:BM:14:ARG:NH2	42:BM:50:ASP:OD2	2.45	0.46
35:BD:106:ALA:HA	35:BD:107:PRO:HD2	1.82	0.46
48:BS:99:LYS:HB3	48:BS:101:TYR:CE2	2.50	0.46
53:BX:87:ASP:CB	53:BX:88:GLY:CA	2.84	0.46
30:B6:34:ARG:CB	30:B6:42:LEU:CD1	2.93	0.46
29:B5:22:ASN:HD22	29:B5:25:ASN:HD22	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AY:8:G:O6	22:AY:9:A:N6	2.49	0.46
33:BA:106:G:H4'	33:BA:337:A:H5''	1.97	0.46
33:BA:337:A:O2'	33:BA:338:G:O4'	2.34	0.46
52:BW:12:VAL:HG21	52:BW:78:LYS:HE2	1.97	0.46
33:BA:675:C:N4	33:BA:676:G:O6	2.48	0.46
1:AA:1068:G:H1	1:AA:1208:U:H3	1.61	0.46
33:BA:1294:A:C3'	33:BA:1295:U:C5'	2.90	0.46
28:B4:18:THR:O	28:B4:21:LYS:NZ	2.48	0.46
35:BD:241:ILE:HD11	35:BD:246:PRO:HA	1.97	0.46
34:BB:98:G:H3'	34:BB:99:A:C8	2.51	0.46
1:AA:343:C:H2'	1:AA:344:A:H8	1.81	0.46
33:BA:282:G:H1'	33:BA:283:G:C8	2.51	0.46
48:BS:50:VAL:HG22	48:BS:64:VAL:HG22	1.98	0.46
21:AX:56:C:C5	38:BG:80:ARG:HD3	2.50	0.46
33:BA:275:A:H62	33:BA:296:G:N2	2.13	0.46
33:BA:1715:C:O2	33:BA:2022:U:O2'	2.23	0.46
38:BG:68:THR:OG1	38:BG:85:ILE:O	2.32	0.46
33:BA:734:C:H42	33:BA:834:C:H4'	1.81	0.46
38:BG:35:VAL:HG13	38:BG:88:LYS:HG3	1.97	0.46
33:BA:2335:U:H3'	33:BA:2336:G:H5''	1.97	0.46
33:BA:837:U:C6	33:BA:837:U:C3'	2.99	0.46
33:BA:2629:A:C2'	33:BA:2630:C:H5'	2.45	0.46
1:AA:243:C:H2'	1:AA:244:G:H8	1.80	0.46
1:AA:54:U:H2'	1:AA:55:A:C8	2.51	0.46
33:BA:1015:G:N2	33:BA:1031:C:OP1	2.44	0.46
43:BN:52:VAL:HG22	43:BN:94:ARG:HH11	1.81	0.46
25:B1:40:THR:HG21	33:BA:61:A:H1'	1.97	0.46
33:BA:647:A:H4'	33:BA:648:G:O5'	2.15	0.46
50:BU:77:LYS:HB2	50:BU:82:VAL:HB	1.97	0.46
53:BX:79:THR:HB	53:BX:95:LYS:H	1.80	0.46
24:B0:37:ARG:CD	24:B0:45:LYS:HG3	2.33	0.46
37:BF:4:VAL:HG12	37:BF:5:ALA:N	2.30	0.46
53:BX:48:THR:HB	53:BX:50:ALA:N	2.31	0.46
1:AA:848:G:O2'	1:AA:849:G:OP1	2.31	0.46
33:BA:615:U:O5'	33:BA:2059:A:N6	2.49	0.46
37:BF:12:SER:HB2	37:BF:13:THR:HB	1.97	0.46
1:AA:415:A:H2'	1:AA:416:G:C8	2.51	0.46
22:AY:15:A:H2'	22:AY:16:A:H5''	1.98	0.46
22:AY:8:G:O5'	22:AY:8:G:H8	1.99	0.46
33:BA:837:U:C6	33:BA:837:U:H3'	2.49	0.46
33:BA:1893:U:OP1	33:BA:2439:G:O2'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BP:29:PHE:HB2	45:BP:105:GLU:OE1	2.16	0.46
1:AA:833:U:H2'	1:AA:834:G:H8	1.81	0.46
35:BD:253:PRO:HG2	35:BD:257:PHE:CG	2.50	0.46
1:AA:510:C:O2	1:AA:558:C:O2'	2.33	0.46
33:BA:753:A:OP1	35:BD:7:LYS:NZ	2.45	0.46
35:BD:243:ARG:NH2	35:BD:247:MET:CB	2.59	0.46
1:AA:66:G:H4'	1:AA:67:A:H5''	1.98	0.46
33:BA:9:U:H2'	33:BA:10:A:H8	1.81	0.46
48:BS:38:GLY:HA2	48:BS:39:ASN:HA	1.56	0.46
47:BR:35:ARG:HA	47:BR:40:ILE:HG13	1.98	0.46
25:B1:31:GLN:O	25:B1:35:GLY:N	2.44	0.46
1:AA:1210:A:H4'	1:AA:1211:U:O5'	2.16	0.46
54:BZ:75:VAL:HG22	54:BZ:89:VAL:HG22	1.98	0.46
49:BT:89:GLU:HG2	50:BU:48:VAL:HG13	1.98	0.46
33:BA:229:A:O2'	33:BA:230:A:OP1	2.33	0.46
33:BA:2009:G:O6	33:BA:2011:U:O4	2.33	0.45
23:AZ:89:ASP:HB2	33:BA:2614:U:C2	2.51	0.45
33:BA:2777:A:H4'	39:BH:67:GLY:HA3	1.97	0.45
33:BA:1788:A:H5''	33:BA:2744:C:H1'	1.97	0.45
49:BT:69:ALA:HB2	49:BT:79:LEU:HD22	1.98	0.45
21:AX:72:C:N4	21:AX:73:G:O6	2.49	0.45
33:BA:1104:U:H2'	33:BA:1105:G:C8	2.51	0.45
33:BA:721:G:C1'	37:BF:74:ARG:HD2	2.46	0.45
47:BR:90:ILE:HA	47:BR:91:SER:HB3	1.98	0.45
36:BE:185:LEU:HD13	48:BS:11:ILE:HD11	1.99	0.45
33:BA:2144:G:O2'	33:BA:2194:G:O6	2.33	0.45
35:BD:94:ILE:HD12	35:BD:104:ILE:HD12	1.98	0.45
36:BE:140:HIS:O	36:BE:142:ARG:N	2.46	0.45
35:BD:58:HIS:HB2	35:BD:213:TRP:HE3	1.81	0.45
33:BA:2648:U:H4'	36:BE:156:LYS:HA	1.97	0.45
33:BA:626:G:H2'	33:BA:627:G:C8	2.51	0.45
33:BA:789:C:H2'	33:BA:790:A:C8	2.51	0.45
9:AI:107:ASP:O	9:AI:109:ARG:N	2.47	0.45
33:BA:928:G:H2'	33:BA:929:G:C8	2.52	0.45
36:BE:15:VAL:HB	36:BE:25:VAL:HG21	1.97	0.45
33:BA:1829:C:P	35:BD:182:ARG:HH22	2.40	0.45
37:BF:67:GLN:HE22	37:BF:74:ARG:CA	2.28	0.45
39:BH:5:GLY:HA2	39:BH:70:ARG:HD3	1.98	0.45
33:BA:338:G:H2'	33:BA:339:A:C8	2.51	0.45
34:BB:11:A:H62	34:BB:68:C:H5'	1.81	0.45
44:BO:106:ASN:O	44:BO:108:GLY:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B1:26:PHE:HE1	52:BW:8:LEU:HB2	1.81	0.45
21:AX:34:G:N3	21:AX:34:G:H2'	2.32	0.45
47:BR:91:SER:HG	47:BR:92:ASP:H	1.61	0.45
42:BM:77:ARG:NH2	42:BM:88:ARG:HH21	2.14	0.45
33:BA:2859:G:H21	33:BA:2908:A:H62	1.64	0.45
46:BQ:104:LEU:HD13	46:BQ:105:GLY:N	2.32	0.45
43:BN:64:ARG:HH12	48:BS:71:VAL:HG21	1.81	0.45
33:BA:377:G:C2	33:BA:378:C:C4	3.05	0.45
22:AY:1:U:H3'	22:AY:2:G:H1'	1.97	0.45
22:AY:8:G:O5'	22:AY:8:G:C8	2.70	0.45
33:BA:1501:U:O2'	33:BA:2878:U:OP1	2.32	0.45
33:BA:2472:C:H2'	33:BA:2473:G:C8	2.50	0.45
1:AA:960:U:H2'	1:AA:961:G:H8	1.81	0.45
33:BA:1242:U:H2'	33:BA:1243:A:C8	2.51	0.45
30:B6:3:ARG:NH1	33:BA:836:A:N1	2.65	0.45
1:AA:1491:U:H2'	1:AA:1492:G:C8	2.52	0.45
35:BD:177:ASN:OD1	35:BD:178:SER:N	2.48	0.45
1:AA:224:U:H2'	1:AA:225:A:C8	2.52	0.45
52:BW:27:THR:HG22	52:BW:80:ILE:HG13	1.98	0.45
43:BN:78:SER:OG	48:BS:74:GLU:OE1	2.34	0.45
40:BJ:89:VAL:HG12	40:BJ:90:VAL:H	1.81	0.45
36:BE:123:ILE:HD11	36:BE:141:ARG:HA	1.98	0.45
33:BA:2784:C:H4'	33:BA:2785:U:OP1	2.17	0.45
33:BA:677:A:OP1	44:BO:64:ARG:NH2	2.49	0.45
33:BA:1754:U:H2'	33:BA:1755:C:C6	2.52	0.45
34:BB:39:A:H3'	34:BB:40:C:H5'	1.98	0.45
33:BA:224:A:H1'	33:BA:236:A:H1'	1.99	0.45
33:BA:1478:G:H2'	33:BA:1479:G:C8	2.52	0.45
33:BA:938:G:H2'	33:BA:939:G:H8	1.81	0.45
39:BH:166:GLU:HA	39:BH:167:GLY:HA2	1.50	0.45
33:BA:2516:G:H2'	33:BA:2517:A:C8	2.52	0.45
29:B5:14:GLU:O	29:B5:16:ASN:ND2	2.49	0.45
33:BA:2009:G:C4	33:BA:2011:U:C6	3.04	0.45
34:BB:76:A:H62	34:BB:96:G:N2	2.07	0.45
33:BA:1108:G:H21	33:BA:1123:A:H62	1.64	0.45
33:BA:2835:A:H5''	36:BE:63:LYS:HD2	1.97	0.45
35:BD:40:LYS:O	35:BD:43:ARG:HG2	2.16	0.45
1:AA:1074:G:H21	1:AA:1199:G:H1'	1.80	0.45
1:AA:960:U:H2'	1:AA:961:G:C8	2.51	0.45
1:AA:956:A:H2'	1:AA:957:G:H8	1.82	0.45
1:AA:1175:G:O2'	1:AA:1178:A:N6	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:1613:C:H2'	33:BA:1614:A:H2'	1.97	0.45
49:BT:60:LEU:O	49:BT:63:THR:OG1	2.30	0.45
50:BU:79:LYS:C	50:BU:80:LYS:CG	2.84	0.45
33:BA:839:G:O4'	33:BA:840:A:C2	2.70	0.45
33:BA:1599:U:H2'	33:BA:1600:G:H5'	1.98	0.45
33:BA:2330:A:H61	33:BA:2344:U:H3	1.64	0.45
1:AA:104:C:H2'	1:AA:105:G:C8	2.52	0.45
42:BM:40:LYS:O	49:BT:67:ALA:HB2	2.17	0.45
35:BD:145:GLU:HG2	35:BD:151:GLY:C	2.37	0.45
1:AA:1421:C:H2'	1:AA:1422:A:C8	2.51	0.45
1:AA:1246:C:O2'	1:AA:1309:G:N2	2.40	0.45
49:BT:49:ASP:O	49:BT:53:LYS:N	2.47	0.45
1:AA:1400:U:H2'	1:AA:1401:G:C8	2.52	0.45
33:BA:2332:G:O2'	38:BG:129:THR:OG1	2.24	0.45
33:BA:719:C:H5'	33:BA:848:G:H22	1.82	0.45
44:BO:117:LEU:HD13	44:BO:119:LYS:O	2.17	0.45
33:BA:2100:A:H2'	33:BA:2101:G:H8	1.81	0.45
1:AA:1013:G:H2'	1:AA:1014:A:H4'	1.99	0.45
33:BA:2923:A:H2'	33:BA:2924:A:C8	2.52	0.45
31:B7:40:GLN:O	31:B7:44:LEU:HG	2.17	0.45
38:BG:67:VAL:HB	38:BG:84:PRO:HB2	1.99	0.45
37:BF:46:GLN:HG2	37:BF:48:THR:HG23	1.99	0.45
33:BA:1298:C:H2'	33:BA:1299:G:C8	2.52	0.45
49:BT:37:GLN:O	49:BT:41:LYS:HG2	2.17	0.45
49:BT:92:ARG:NH1	49:BT:93:LYS:HB2	2.32	0.45
1:AA:1544:A:H8	1:AA:1544:A:C5'	2.29	0.45
33:BA:1755:C:H2'	33:BA:1756:U:C6	2.52	0.45
49:BT:42:SER:O	49:BT:46:ALA:N	2.50	0.45
1:AA:842:U:HO2'	1:AA:843:U:P	2.39	0.45
33:BA:2349:A:O2'	33:BA:2362:A:N6	2.50	0.45
35:BD:81:VAL:HA	35:BD:92:ALA:HA	1.99	0.45
33:BA:2757:U:O2	36:BE:191:ASN:ND2	2.49	0.45
33:BA:356:G:H2'	33:BA:357:G:H8	1.82	0.45
33:BA:1187:U:OP2	42:BM:66:THR:OG1	2.35	0.45
1:AA:307:G:N2	1:AA:574:U:O2	2.50	0.45
1:AA:974:A:H5''	1:AA:1207:A:O3'	2.17	0.45
34:BB:30:C:H42	34:BB:48:G:H1	1.63	0.45
1:AA:73:C:H2'	1:AA:74:A:C8	2.52	0.45
50:BU:4:ILE:O	50:BU:38:VAL:HG13	2.17	0.45
33:BA:1219:C:H3'	33:BA:1220:G:H4'	1.98	0.45
53:BX:86:GLU:HG3	53:BX:87:ASP:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BF:71:GLY:O	37:BF:72:ARG:HG2	2.16	0.44
33:BA:1848:A:H5''	35:BD:160:THR:HG21	1.99	0.44
33:BA:2718:U:H5'	33:BA:2897:G:H22	1.82	0.44
45:BP:67:LYS:HD2	45:BP:105:GLU:OE2	2.17	0.44
1:AA:1257:A:H2	1:AA:1298:A:H62	1.65	0.44
33:BA:17:G:H4'	49:BT:25:PHE:HE1	1.83	0.44
33:BA:825:G:O6	33:BA:833:C:N3	2.50	0.44
1:AA:1111:A:H4'	1:AA:1112:A:O5'	2.18	0.44
1:AA:1495:U:H2'	1:AA:1496:G:H8	1.81	0.44
40:BJ:4:ALA:O	40:BJ:7:THR:OG1	2.25	0.44
1:AA:1317:C:OP1	13:AM:97:VAL:N	2.48	0.44
33:BA:609:C:C5	50:BU:79:LYS:HE2	2.51	0.44
22:AY:13:G:C8	22:AY:13:G:OP2	2.70	0.44
34:BB:98:G:H3'	34:BB:99:A:H8	1.82	0.44
27:B3:55:ARG:HA	27:B3:56:VAL:HA	1.55	0.44
42:BM:14:ARG:NH2	42:BM:50:ASP:O	2.50	0.44
1:AA:523:C:H2'	1:AA:524:G:H8	1.83	0.44
42:BM:5:PRO:HB3	49:BT:61:TRP:HE1	1.82	0.44
33:BA:377:G:C2'	33:BA:378:C:H6	2.11	0.44
33:BA:1364:C:N3	51:BV:86:ARG:CZ	2.79	0.44
22:AY:13:G:O2'	22:AY:14:G:C6	2.70	0.44
40:BJ:58:THR:HG21	40:BJ:82:ILE:O	2.18	0.44
33:BA:1003:A:N1	33:BA:2487:U:H4'	2.32	0.44
45:BP:57:TYR:CE2	45:BP:113:VAL:HG13	2.53	0.44
33:BA:1455:C:O2'	33:BA:1456:A:OP1	2.27	0.44
53:BX:32:ARG:HB3	53:BX:62:PRO:HB2	1.99	0.44
1:AA:328:G:H2'	1:AA:329:A:C8	2.52	0.44
22:AY:3:U:OP2	22:AY:3:U:C5	2.70	0.44
38:BG:79:LEU:HD23	38:BG:83:MET:HB2	1.99	0.44
21:AX:18:G:O2'	21:AX:57:G:N2	2.51	0.44
1:AA:716:U:H2'	1:AA:717:G:H8	1.81	0.44
1:AA:1385:U:H2'	1:AA:1386:A:C8	2.52	0.44
41:BK:131:THR:O	41:BK:134:SER:OG	2.24	0.44
33:BA:2078:A:N6	33:BA:2647:G:O6	2.51	0.44
33:BA:1619:A:H2'	33:BA:1620:A:C8	2.52	0.44
1:AA:58:U:H2'	1:AA:59:G:C8	2.53	0.44
40:BJ:32:GLY:HA2	40:BJ:108:ILE:HD11	1.99	0.44
40:BJ:84:PHE:HA	40:BJ:116:LYS:NZ	2.32	0.44
33:BA:823:G:H2'	33:BA:824:G:OP1	2.18	0.44
33:BA:29:U:O2	33:BA:1255:G:O2'	2.36	0.44
1:AA:1469:C:H2'	1:AA:1470:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BV:3:ALA:HB3	51:BV:107:VAL:HB	1.99	0.44
33:BA:406:G:H2'	33:BA:407:A:C8	2.53	0.44
1:AA:754:U:OP1	1:AA:861:U:O2'	2.29	0.44
33:BA:2540:U:HO2'	36:BE:139:TYR:HH	1.57	0.44
33:BA:938:G:H2'	33:BA:939:G:C8	2.53	0.44
33:BA:897:G:O6	33:BA:974:A:N6	2.50	0.44
42:BM:124:ASN:HB3	42:BM:126:TYR:HE2	1.83	0.44
33:BA:1817:C:OP1	35:BD:221:ARG:NH1	2.50	0.44
35:BD:84:ASP:HB2	35:BD:91:ILE:HG13	2.00	0.44
36:BE:84:ARG:HA	36:BE:85:GLY:HA2	1.61	0.44
9:AI:104:LEU:O	9:AI:106:ARG:N	2.38	0.44
33:BA:1886:G:H21	33:BA:1914:A:H62	1.65	0.44
34:BB:36:C:H2'	34:BB:37:A:O4'	2.17	0.44
39:BH:19:LEU:HD21	39:BH:46:VAL:HG23	2.00	0.44
33:BA:2010:A:H3'	33:BA:2011:U:C5'	2.47	0.44
46:BQ:27:ASN:C	46:BQ:29:ARG:H	2.20	0.44
1:AA:505:G:N2	1:AA:507:A:OP2	2.51	0.44
21:AX:36:C:N4	21:AX:37:A:H62	2.16	0.44
1:AA:1335:U:H2'	1:AA:1336:G:C8	2.51	0.44
49:BT:46:ALA:O	49:BT:50:ARG:HG3	2.18	0.44
1:AA:1502:A:H5'	1:AA:1503:A:OP2	2.18	0.44
26:B2:19:GLN:O	26:B2:22:THR:OG1	2.22	0.44
31:B7:7:HIS:HE2	33:BA:254:A:P	2.40	0.44
49:BT:10:THR:O	49:BT:14:ARG:HG2	2.18	0.44
20:AT:6:SER:O	20:AT:8:ILE:N	2.44	0.44
28:B4:7:ARG:HB3	33:BA:2046:U:O2	2.17	0.44
33:BA:302:A:H2'	33:BA:303:G:C8	2.52	0.44
33:BA:794:U:H2'	33:BA:795:G:OP1	2.17	0.44
22:AY:13:G:O2'	22:AY:14:G:C5	2.71	0.44
1:AA:1074:G:N2	1:AA:1199:G:H1'	2.32	0.44
33:BA:2164:A:H62	33:BA:2185:G:H21	1.66	0.44
53:BX:9:VAL:HG13	53:BX:69:MET:H	1.82	0.44
36:BE:150:ASP:N	36:BE:151:PRO:HD2	2.33	0.44
33:BA:2221:C:H2'	33:BA:2222:C:H5'	2.00	0.44
33:BA:1029:A:N6	33:BA:1030:G:C6	2.86	0.44
40:BJ:71:GLY:O	40:BJ:73:ASN:N	2.45	0.44
33:BA:1364:C:C4	51:BV:86:ARG:NH1	2.86	0.44
33:BA:1659:A:N7	33:BA:1660:C:H5	2.15	0.44
33:BA:252:C:OP2	33:BA:2423:C:O2'	2.26	0.44
33:BA:1046:A:H62	33:BA:1200:G:H2'	1.83	0.44
33:BA:1696:G:O5'	46:BQ:35:THR:OG1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:279:A:H2'	33:BA:280:G:C8	2.52	0.44
13:AM:41:GLU:CA	13:AM:42:ASP:O	2.66	0.44
33:BA:1305:A:HO2'	51:BV:15:ARG:HH22	1.64	0.44
47:BR:65:VAL:HB	47:BR:68:THR:H	1.82	0.43
49:BT:103:LEU:HA	49:BT:104:THR:HA	1.76	0.43
33:BA:1348:G:H21	33:BA:1656:C:H5'	1.83	0.43
23:AZ:89:ASP:HB2	33:BA:2614:U:O2	2.18	0.43
33:BA:2070:U:H2'	33:BA:2071:A:H8	1.82	0.43
1:AA:126:G:H1	1:AA:241:C:N4	2.16	0.43
38:BG:107:SER:HB2	38:BG:137:ILE:HG22	1.99	0.43
38:BG:108:LEU:N	38:BG:109:PRO:HD2	2.32	0.43
20:AT:67:VAL:H	20:AT:68:HIS:CA	2.30	0.43
34:BB:79:C:N4	34:BB:80:G:O6	2.51	0.43
22:AY:6:A:H2'	22:AY:7:C:H6	1.83	0.43
48:BS:5:GLN:HB2	48:BS:8:ILE:HB	1.99	0.43
42:BM:77:ARG:NH1	42:BM:88:ARG:HE	2.15	0.43
33:BA:1023:G:H5'	49:BT:55:ARG:NH1	2.33	0.43
37:BF:10:ASN:H	37:BF:12:SER:HB3	1.83	0.43
31:B7:26:HIS:CE1	31:B7:48:ALA:HB2	2.54	0.43
23:AZ:86:ASP:O	23:AZ:87:GLU:HB2	2.18	0.43
47:BR:65:VAL:HG21	47:BR:68:THR:HA	2.00	0.43
33:BA:377:G:C2	33:BA:378:C:C5	3.06	0.43
37:BF:37:ILE:HD13	44:BO:6:LEU:HD21	2.01	0.43
33:BA:2476:G:N2	33:BA:2479:A:OP2	2.51	0.43
35:BD:207:LYS:HE2	35:BD:209:GLY:HA3	2.01	0.43
33:BA:199:A:H62	33:BA:878:G:N2	2.16	0.43
52:BW:12:VAL:HG11	52:BW:78:LYS:NZ	2.34	0.43
33:BA:1023:G:H5'	49:BT:55:ARG:HH12	1.83	0.43
33:BA:1374:C:OP1	52:BW:65:ARG:NH1	2.51	0.43
1:AA:646:U:H2'	1:AA:647:G:H8	1.83	0.43
43:BN:8:LEU:HD22	43:BN:82:ASN:HB3	2.00	0.43
44:BO:125:ALA:HB3	44:BO:128:PHE:CZ	2.53	0.43
24:B0:23:ASN:HB2	24:B0:24:ALA:HA	2.00	0.43
33:BA:2862:A:H2'	33:BA:2863:G:C8	2.53	0.43
33:BA:2152:A:H2'	33:BA:2153:G:H8	1.82	0.43
1:AA:500:A:H2'	1:AA:501:A:H8	1.83	0.43
41:BK:15:ALA:HA	41:BK:46:THR:HG21	2.00	0.43
33:BA:507:A:H62	33:BA:516:G:N2	2.12	0.43
33:BA:879:G:H2'	33:BA:880:C:C6	2.53	0.43
25:B1:2:LYS:HE2	33:BA:78:U:H5''	2.00	0.43
47:BR:35:ARG:HB3	47:BR:100:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:2906:U:O4	33:BA:2907:A:N6	2.52	0.43
33:BA:1248:C:H2'	33:BA:1248:C:O2	2.17	0.43
1:AA:1516:U:N3	1:AA:1532:U:OP1	2.44	0.43
9:AI:42:ALA:O	9:AI:44:LEU:N	2.45	0.43
35:BD:179:GLY:HA3	35:BD:275:LYS:HD3	1.99	0.43
49:BT:114:LYS:HA	49:BT:117:LEU:HD12	1.99	0.43
33:BA:666:G:H4'	33:BA:667:A:C5'	2.48	0.43
35:BD:245:SER:HA	35:BD:246:PRO:HD2	1.78	0.43
45:BP:36:ALA:HB1	45:BP:127:ILE:HG21	2.00	0.43
33:BA:1438:C:H2'	33:BA:1439:U:C6	2.53	0.43
47:BR:72:SER:O	47:BR:75:THR:OG1	2.22	0.43
1:AA:1066:U:H2'	1:AA:1067:G:C8	2.52	0.43
33:BA:1242:U:H2'	33:BA:1243:A:H8	1.83	0.43
38:BG:69:ARG:HA	38:BG:84:PRO:HA	2.00	0.43
38:BG:111:VAL:HG22	38:BG:137:ILE:HG12	1.99	0.43
33:BA:966:U:H4'	34:BB:79:C:H4'	1.99	0.43
36:BE:117:LYS:HG3	36:BE:164:MET:HE3	2.01	0.43
1:AA:1063:G:N7	1:AA:1209:C:H5''	2.34	0.43
1:AA:930:U:H2'	1:AA:931:U:C6	2.54	0.43
33:BA:1932:G:H2'	33:BA:1933:G:H8	1.83	0.43
33:BA:2327:A:H62	33:BA:2347:G:H8	1.67	0.43
33:BA:2346:C:N4	33:BA:2347:G:N7	2.67	0.43
26:B2:10:ARG:HD3	33:BA:1034:A:OP1	2.18	0.43
33:BA:1105:G:H2'	33:BA:1106:U:C5	2.54	0.43
37:BF:129:LEU:HD12	37:BF:195:THR:HG22	2.00	0.43
38:BG:64:LYS:HA	38:BG:65:PRO:HD2	1.91	0.43
33:BA:1783:C:H5'	48:BS:102:TYR:CZ	2.54	0.43
33:BA:1108:G:H1	33:BA:1122:C:H42	1.66	0.43
1:AA:643:C:H2'	1:AA:644:A:C8	2.54	0.43
1:AA:734:G:OP1	1:AA:863:G:N2	2.41	0.43
1:AA:1283:A:HO2'	1:AA:1284:A:H8	1.67	0.43
33:BA:300:G:N7	33:BA:468:C:H2'	2.33	0.43
33:BA:2029:G:H2'	33:BA:2030:A:H8	1.84	0.43
25:B1:52:ARG:O	25:B1:56:VAL:HG23	2.19	0.43
1:AA:609:U:H2'	1:AA:610:G:C8	2.53	0.43
33:BA:720:C:N4	33:BA:721:G:O6	2.51	0.43
38:BG:135:GLN:HE22	38:BG:150:ARG:N	2.11	0.43
33:BA:683:A:O2'	33:BA:684:G:O4'	2.24	0.43
33:BA:365:U:H4'	37:BF:165:LEU:O	2.19	0.43
33:BA:2577:G:O2'	43:BN:4:GLN:OE1	2.36	0.43
33:BA:2468:A:H8	33:BA:2468:A:H5'	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:181:G:HO2'	1:AA:182:U:H6	1.65	0.43
1:AA:1403:A:N6	1:AA:1511:C:H5'	2.34	0.43
33:BA:1818:A:H5''	35:BD:220:VAL:HA	2.01	0.43
1:AA:398:C:H2'	1:AA:399:G:C8	2.54	0.43
1:AA:950:C:H2'	1:AA:951:G:C8	2.54	0.43
33:BA:746:A:H4'	33:BA:1679:A:C6	2.54	0.43
33:BA:719:C:H5'	33:BA:848:G:N2	2.33	0.43
44:BO:23:ILE:HG21	50:BU:81:ASN:O	2.16	0.43
41:BK:98:ALA:HB3	41:BK:137:ILE:HG12	2.00	0.43
19:AS:81:LYS:N	19:AS:82:GLY:HA2	2.33	0.43
1:AA:609:U:H2'	1:AA:610:G:H8	1.83	0.43
1:AA:398:C:H2'	1:AA:399:G:H8	1.83	0.43
38:BG:32:GLU:HG3	47:BR:2:ILE:HD12	2.01	0.43
1:AA:551:U:H2'	1:AA:552:G:C8	2.53	0.43
33:BA:2038:G:H1'	46:BQ:110:ASP:O	2.19	0.43
33:BA:2405:A:N6	33:BA:2406:A:C6	2.87	0.43
25:B1:34:THR:HG22	25:B1:36:GLN:HG3	2.01	0.43
33:BA:661:A:O2'	37:BF:40:GLN:OE1	2.23	0.43
33:BA:373:A:N6	53:BX:15:LYS:H	2.17	0.43
35:BD:171:TYR:HB3	35:BD:184:ILE:O	2.18	0.43
33:BA:1018:G:H3'	33:BA:1019:A:H5''	2.00	0.43
54:BZ:80:PHE:HB2	54:BZ:84:ARG:HB3	2.01	0.43
46:BQ:17:LEU:CD2	46:BQ:39:GLU:OE2	2.67	0.43
1:AA:995:C:H2'	1:AA:996:A:C8	2.54	0.43
50:BU:65:GLN:HG2	50:BU:93:THR:HG23	2.00	0.43
1:AA:473:G:N2	1:AA:478:G:O6	2.52	0.43
33:BA:1759:U:O4	33:BA:1774:A:N7	2.52	0.43
35:BD:29:PRO:HB3	35:BD:63:ARG:NE	2.31	0.43
27:B3:1:MET:N	34:BB:38:U:O4	2.43	0.43
33:BA:1340:A:N6	33:BA:1686:A:C2	2.86	0.43
1:AA:95:U:H2'	1:AA:96:G:H8	1.83	0.43
33:BA:970:A:H4'	54:BZ:37:GLN:HE22	1.83	0.43
49:BT:64:ARG:HD2	49:BT:97:ASP:OD2	2.18	0.43
33:BA:2610:G:H22	33:BA:2639:C:H2'	1.84	0.43
49:BT:103:LEU:CD1	49:BT:104:THR:HA	2.38	0.42
31:B7:8:ARG:HG2	33:BA:249:C:H41	1.84	0.42
33:BA:1813:A:H4'	33:BA:1814:A:O5'	2.18	0.42
42:BM:17:LEU:HD23	42:BM:139:GLU:HB2	2.01	0.42
33:BA:647:A:C2	33:BA:672:C:H4'	2.54	0.42
45:BP:43:THR:HA	45:BP:94:VAL:HG22	2.01	0.42
33:BA:2648:U:H5'	36:BE:156:LYS:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:625:C:H2'	33:BA:626:G:C8	2.54	0.42
1:AA:266:A:H2'	1:AA:267:G:C8	2.54	0.42
33:BA:709:G:H5''	44:BO:16:ARG:HA	2.01	0.42
33:BA:1355:U:H5'	33:BA:1431:G:H1'	2.01	0.42
40:BJ:119:THR:OG1	40:BJ:120:VAL:N	2.52	0.42
43:BN:7:ARG:HA	43:BN:20:LEU:HA	2.01	0.42
33:BA:125:A:N6	33:BA:126:A:N1	2.67	0.42
1:AA:989:C:OP1	1:AA:1232:C:N4	2.52	0.42
1:AA:1547:U:H6	1:AA:1547:U:O5'	2.01	0.42
37:BF:67:GLN:HE22	37:BF:74:ARG:HA	1.84	0.42
33:BA:839:G:H4'	33:BA:840:A:C2	2.54	0.42
49:BT:92:ARG:CG	49:BT:94:MET:HG2	2.49	0.42
33:BA:673:A:N7	44:BO:76:VAL:HG11	2.34	0.42
36:BE:49:ILE:HD12	36:BE:86:VAL:HG21	2.00	0.42
33:BA:2721:C:O2	33:BA:2872:U:O2'	2.31	0.42
38:BG:169:LEU:O	38:BG:173:VAL:HG23	2.19	0.42
33:BA:527:A:H1'	53:BX:41:VAL:HG11	2.01	0.42
42:BM:45:TYR:H	49:BT:64:ARG:NE	2.17	0.42
33:BA:2336:G:OP1	33:BA:2336:G:N2	2.49	0.42
38:BG:106:VAL:HG11	38:BG:139:PRO:HG3	2.01	0.42
35:BD:235:GLY:HA3	35:BD:239:ALA:HB2	2.00	0.42
46:BQ:107:ARG:HG2	46:BQ:109:GLY:H	1.84	0.42
33:BA:2801:C:C2	33:BA:2802:U:C5	3.07	0.42
33:BA:2864:G:O6	33:BA:2902:A:N6	2.50	0.42
1:AA:1231:G:OP2	1:AA:1331:C:N4	2.48	0.42
24:B0:42:GLY:HA2	24:B0:43:LYS:HA	1.64	0.42
33:BA:1250:G:H5''	33:BA:1252:G:O4'	2.18	0.42
33:BA:1133:G:H1	33:BA:1148:C:N4	2.17	0.42
21:AX:34:G:C2'	21:AX:35:U:H5''	2.50	0.42
33:BA:678:A:O3'	44:BO:68:ASN:ND2	2.32	0.42
33:BA:1003:A:C2	33:BA:2487:U:H4'	2.54	0.42
33:BA:275:A:N6	33:BA:296:G:H21	2.17	0.42
45:BP:14:ARG:HD3	45:BP:41:TRP:HH2	1.85	0.42
37:BF:11:GLY:N	37:BF:12:SER:HB3	2.34	0.42
33:BA:278:A:H2'	33:BA:279:A:C8	2.54	0.42
52:BW:65:ARG:HB3	52:BW:70:THR:HG22	2.00	0.42
33:BA:1983:G:O2'	33:BA:1985:U:O4	2.29	0.42
33:BA:1694:G:H2'	33:BA:1695:A:C8	2.54	0.42
35:BD:136:PRO:HG2	35:BD:139:THR:HG21	2.01	0.42
1:AA:739:G:C5	1:AA:740:G:H1'	2.53	0.42
28:B4:35:GLU:HA	28:B4:36:MET:HA	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:1231:G:OP1	44:BO:30:THR:OG1	2.36	0.42
35:BD:185:LEU:HD12	35:BD:186:SER:N	2.34	0.42
33:BA:2262:A:H2'	33:BA:2263:G:C8	2.54	0.42
1:AA:326:G:H2'	1:AA:327:G:H8	1.84	0.42
1:AA:149:U:H2'	1:AA:150:A:H8	1.84	0.42
29:B5:6:THR:HG22	29:B5:18:ILE:HG12	2.00	0.42
39:BH:21:ASP:HA	39:BH:22:ASN:HA	1.85	0.42
33:BA:1065:U:C2	33:BA:1188:A:N6	2.88	0.42
45:BP:104:PHE:HE2	45:BP:125:LEU:HD11	1.83	0.42
33:BA:970:A:O2'	54:BZ:37:GLN:NE2	2.52	0.42
1:AA:1525:C:H2'	1:AA:1526:G:H8	1.83	0.42
31:B7:26:HIS:ND1	31:B7:46:LYS:O	2.50	0.42
33:BA:1345:U:O2'	33:BA:1346:A:H5''	2.20	0.42
27:B3:18:CYS:SG	27:B3:20:ASN:ND2	2.93	0.42
1:AA:119:C:H4'	1:AA:120:A:O5'	2.17	0.42
46:BQ:51:GLY:HA2	46:BQ:84:PHE:CE1	2.54	0.42
22:AY:3:U:O5'	22:AY:3:U:C6	2.70	0.42
24:B0:38:ILE:HG22	24:B0:39:LEU:N	2.34	0.42
33:BA:513:A:O5'	33:BA:513:A:H8	2.01	0.42
33:BA:1808:U:O2	33:BA:1812:A:N6	2.53	0.42
44:BO:75:ALA:HA	44:BO:76:VAL:HA	1.76	0.42
1:AA:1081:C:H2'	1:AA:1082:G:H8	1.85	0.42
1:AA:104:C:H2'	1:AA:105:G:H8	1.85	0.42
33:BA:1305:A:O2'	33:BA:1306:G:O5'	2.29	0.42
50:BU:22:ILE:O	50:BU:93:THR:N	2.40	0.42
45:BP:35:GLN:HE21	45:BP:100:GLY:HA2	1.85	0.42
33:BA:20:C:H2'	33:BA:21:A:C8	2.55	0.42
33:BA:2769:A:N6	33:BA:2770:A:N6	2.67	0.42
40:BJ:78:GLY:N	40:BJ:79:PRO:HD2	2.34	0.42
33:BA:2011:U:O2'	33:BA:2012:C:H5'	2.20	0.42
29:B5:22:ASN:HD22	29:B5:25:ASN:ND2	2.18	0.42
33:BA:1362:G:H3'	33:BA:1363:G:H5''	2.01	0.42
33:BA:2488:A:N6	33:BA:2523:G:C2	2.88	0.42
33:BA:2746:G:O2'	48:BS:97:ARG:NH1	2.52	0.42
27:B3:2:LYS:NZ	34:BB:40:C:OP1	2.52	0.42
34:BB:40:C:HO2'	34:BB:41:C:C5'	2.32	0.42
33:BA:1887:G:HO2'	33:BA:1888:A:H8	1.63	0.42
49:BT:59:LYS:O	49:BT:63:THR:HG23	2.20	0.42
1:AA:974:A:N6	1:AA:975:A:N6	2.67	0.42
1:AA:73:C:H2'	1:AA:74:A:H8	1.85	0.42
33:BA:1224:A:H2'	33:BA:1225:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:2812:A:HO2'	33:BA:2813:U:P	2.43	0.42
33:BA:2868:G:H2'	33:BA:2869:A:H8	1.85	0.42
30:B6:17:GLY:O	30:B6:20:SER:OG	2.29	0.42
40:BJ:123:VAL:O	40:BJ:124:LYS:HB2	2.19	0.42
30:B6:34:ARG:HB3	30:B6:42:LEU:CD1	2.50	0.42
22:AY:10:U:C6	22:AY:10:U:OP2	2.73	0.42
22:AY:8:G:O6	22:AY:9:A:C6	2.72	0.42
33:BA:1848:A:OP1	35:BD:157:SER:OG	2.28	0.42
33:BA:787:C:N4	33:BA:804:G:H1	2.15	0.42
1:AA:1508:U:OP2	22:AY:17:G:O2'	2.37	0.42
33:BA:2358:A:N6	33:BA:2359:G:C6	2.88	0.42
33:BA:1398:A:H62	33:BA:1411:U:H3	1.67	0.42
1:AA:1012:U:H2'	1:AA:1013:G:O4'	2.20	0.42
33:BA:1694:G:H2'	33:BA:1695:A:H8	1.85	0.42
35:BD:72:ASP:HB2	35:BD:119:GLY:HA2	2.02	0.42
33:BA:2825:C:H3'	33:BA:2826:A:H8	1.85	0.42
1:AA:1473:C:H2'	1:AA:1474:G:H8	1.84	0.42
33:BA:2134:A:H2'	33:BA:2135:G:C8	2.55	0.42
43:BN:10:VAL:HG12	43:BN:12:ASP:H	1.85	0.42
33:BA:1407:G:H2'	33:BA:1408:G:H8	1.84	0.42
33:BA:509:C:N4	33:BA:510:G:O6	2.53	0.42
1:AA:754:U:H2'	1:AA:755:G:C8	2.54	0.42
35:BD:174:VAL:HG21	35:BD:184:ILE:HD12	2.02	0.42
33:BA:1108:G:H2'	33:BA:1109:G:C8	2.53	0.42
34:BB:41:C:O2'	34:BB:42:G:H5'	2.19	0.42
53:BX:4:LYS:N	53:BX:92:ARG:HH22	2.17	0.42
42:BM:4:THR:N	42:BM:5:PRO:HD2	2.35	0.42
1:AA:1434:A:O2'	1:AA:1435:A:H5''	2.20	0.42
42:BM:128:GLY:HA2	42:BM:129:SER:HA	1.68	0.42
31:B7:17:THR:HG21	31:B7:23:LYS:HG3	2.01	0.42
33:BA:259:A:H2'	33:BA:260:A:C8	2.54	0.42
1:AA:280:C:H2'	1:AA:281:A:H8	1.84	0.42
44:BO:33:LYS:HB3	44:BO:40:ALA:HA	2.01	0.42
1:AA:875:A:H5'	1:AA:1088:U:C5	2.55	0.42
24:B0:45:LYS:HE3	24:B0:46:LYS:HE3	2.02	0.42
33:BA:377:G:O2'	33:BA:378:C:OP1	2.38	0.42
37:BF:66:ARG:CD	37:BF:70:THR:HG23	2.49	0.42
33:BA:1659:A:N6	51:BV:91:GLY:HA2	2.35	0.42
33:BA:2295:A:N6	33:BA:2302:A:H62	2.10	0.42
38:BG:42:ASP:HB3	38:BG:45:GLN:H	1.84	0.42
33:BA:1433:U:H4'	33:BA:1648:A:H4'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:694:G:H2'	33:BA:695:G:C8	2.55	0.42
29:B5:14:GLU:HG2	29:B5:16:ASN:H	1.84	0.42
33:BA:1298:C:H2'	33:BA:1299:G:H8	1.85	0.42
33:BA:2181:C:H2'	33:BA:2182:G:C8	2.55	0.42
44:BO:7:LYS:HA	44:BO:8:PRO:HD3	1.92	0.42
45:BP:7:VAL:HG12	45:BP:9:TYR:H	1.84	0.42
47:BR:49:ASN:HB3	47:BR:51:VAL:HG23	2.02	0.42
35:BD:19:SER:HB3	35:BD:203:ILE:HD11	2.02	0.42
29:B5:12:CYS:SG	29:B5:38:ARG:HD3	2.60	0.42
33:BA:2089:A:H1'	33:BA:2531:G:H1'	2.01	0.42
33:BA:2042:A:O2'	51:BV:94:SER:HB3	2.20	0.42
46:BQ:9:THR:O	46:BQ:13:ARG:HG3	2.20	0.42
35:BD:144:ILE:HG21	35:BD:184:ILE:HD13	2.01	0.42
36:BE:201:THR:HG21	36:BE:203:LYS:HG3	1.99	0.42
33:BA:731:G:N2	33:BA:835:A:OP2	2.47	0.42
33:BA:933:C:H2'	33:BA:934:U:H5'	2.02	0.42
40:BJ:53:LYS:HB3	40:BJ:55:TYR:CD2	2.54	0.42
33:BA:1093:G:N2	33:BA:1157:A:H62	2.17	0.42
51:BV:36:LEU:HB3	51:BV:44:SER:HB2	2.02	0.42
1:AA:126:G:H1	1:AA:241:C:H42	1.68	0.42
1:AA:833:U:H2'	1:AA:834:G:C8	2.55	0.42
1:AA:74:A:H2'	1:AA:75:G:O4'	2.20	0.42
33:BA:511:U:H2'	33:BA:512:G:O4'	2.20	0.42
33:BA:2607:G:OP1	33:BA:2643:A:N6	2.53	0.42
33:BA:1005:A:H2'	33:BA:1006:A:C8	2.55	0.42
48:BS:107:ARG:HA	48:BS:108:GLY:HA2	1.59	0.42
51:BV:79:GLY:H	51:BV:101:SER:HA	1.84	0.42
33:BA:2874:G:N2	33:BA:2891:G:H1'	2.35	0.42
24:B0:7:ILE:HD12	24:B0:49:VAL:HG23	2.00	0.41
37:BF:75:GLN:NE2	37:BF:82:GLN:HE22	2.14	0.41
33:BA:2186:G:O2'	33:BA:2187:A:O4'	2.30	0.41
33:BA:2296:A:H5''	33:BA:2297:A:H5'	2.01	0.41
35:BD:69:ARG:NH1	35:BD:104:ILE:HD13	2.35	0.41
33:BA:2342:C:H2'	33:BA:2343:A:C8	2.55	0.41
33:BA:908:A:H2'	33:BA:909:G:O4'	2.20	0.41
1:AA:345:G:H2'	1:AA:346:A:H8	1.84	0.41
33:BA:614:G:H2'	33:BA:2059:A:N7	2.35	0.41
1:AA:510:C:H2'	1:AA:511:C:C6	2.55	0.41
33:BA:2468:A:H4'	33:BA:2469:C:O5'	2.19	0.41
4:AD:25:GLU:O	4:AD:27:GLU:N	2.45	0.41
33:BA:2157:C:H2'	33:BA:2158:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:146:G:H2'	1:AA:147:G:C8	2.55	0.41
36:BE:119:PHE:CE1	36:BE:162:GLY:HA2	2.55	0.41
33:BA:430:C:C2	33:BA:438:A:N6	2.87	0.41
43:BN:66:LYS:N	43:BN:82:ASN:OD1	2.48	0.41
1:AA:478:G:H2'	1:AA:479:G:C8	2.55	0.41
33:BA:978:A:O3'	33:BA:979:U:O4'	2.39	0.41
1:AA:1160:A:HO2'	1:AA:1161:A:H8	1.68	0.41
1:AA:815:C:N4	1:AA:816:A:H62	2.19	0.41
33:BA:1626:U:H2'	33:BA:1627:A:H8	1.84	0.41
1:AA:35:A:N6	1:AA:559:G:O6	2.53	0.41
37:BF:128:ASP:OD1	37:BF:130:THR:HG23	2.20	0.41
33:BA:58:G:H2'	33:BA:59:G:C8	2.55	0.41
35:BD:96:TYR:HE2	35:BD:102:ARG:HB2	1.85	0.41
33:BA:1938:C:H2'	33:BA:1939:G:C8	2.55	0.41
1:AA:502:C:H2'	1:AA:503:C:C6	2.55	0.41
41:BK:110:GLU:HA	41:BK:113:MET:HG2	2.03	0.41
41:BK:54:ILE:HG23	41:BK:71:LYS:O	2.21	0.41
22:AY:4:G:C3'	22:AY:5:A:H5'	2.46	0.41
50:BU:90:GLN:HA	50:BU:91:PRO:HD2	1.94	0.41
28:B4:16:ARG:HH12	33:BA:1304:G:H5''	1.85	0.41
33:BA:1056:A:H1'	33:BA:1199:C:H1'	2.02	0.41
36:BE:139:TYR:OH	36:BE:142:ARG:O	2.37	0.41
33:BA:2708:A:H2	36:BE:191:ASN:HD22	1.67	0.41
21:AX:58:A:N6	21:AX:61:C:O2	2.53	0.41
37:BF:187:VAL:HG12	44:BO:3:LEU:HB2	2.01	0.41
1:AA:1483:G:H2'	1:AA:1484:G:C8	2.55	0.41
2:AB:103:ASN:O	2:AB:105:GLU:N	2.53	0.41
33:BA:574:A:H62	33:BA:2072:C:C5'	2.34	0.41
33:BA:1107:U:C6	33:BA:1116:A:H4'	2.55	0.41
45:BP:11:ARG:HE	45:BP:87:LYS:HD3	1.85	0.41
28:B4:3:VAL:H	33:BA:2085:G:H21	1.67	0.41
33:BA:377:G:O2'	33:BA:378:C:P	2.78	0.41
33:BA:2123:A:N1	33:BA:2224:U:O2	2.54	0.41
21:AX:71:C:C6	21:AX:71:C:H5''	2.44	0.41
48:BS:51:ILE:HG23	48:BS:100:LEU:N	2.36	0.41
37:BF:11:GLY:HA3	37:BF:12:SER:HA	1.93	0.41
33:BA:825:G:H5''	35:BD:48:LYS:HE3	2.02	0.41
1:AA:1430:U:H2'	1:AA:1431:U:C6	2.56	0.41
33:BA:1782:G:H4'	48:BS:96:ARG:HG2	2.03	0.41
1:AA:530:G:H1	1:AA:537:C:H42	1.69	0.41
1:AA:912:G:H2'	1:AA:913:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:2843:G:H2'	33:BA:2844:A:C8	2.56	0.41
38:BG:127:ASN:N	47:BR:1:MET:SD	2.86	0.41
37:BF:143:LEU:O	37:BF:148:VAL:HG22	2.21	0.41
33:BA:91:A:H5''	33:BA:92:G:H8	1.86	0.41
1:AA:861:U:C4	1:AA:862:A:N6	2.87	0.41
33:BA:1905:A:N6	33:BA:1906:A:C6	2.88	0.41
33:BA:251:G:O5'	33:BA:252:C:H5''	2.20	0.41
28:B4:13:LYS:HA	28:B4:16:ARG:HE	1.85	0.41
33:BA:1199:C:H2'	33:BA:1200:G:O4'	2.19	0.41
34:BB:55:A:H5'	38:BG:24:SER:HB3	2.03	0.41
33:BA:1525:G:H2'	33:BA:1526:G:C8	2.56	0.41
39:BH:28:LYS:HA	39:BH:33:GLU:HG2	2.02	0.41
37:BF:88:VAL:O	37:BF:90:PHE:N	2.54	0.41
33:BA:2440:A:H2'	33:BA:2441:A:C8	2.55	0.41
33:BA:1262:C:H2'	33:BA:1263:G:H8	1.86	0.41
33:BA:1813:A:O2'	33:BA:1814:A:OP2	2.35	0.41
37:BF:167:ALA:HB1	37:BF:173:VAL:HG11	2.01	0.41
33:BA:2329:A:N6	33:BA:2330:A:N6	2.68	0.41
38:BG:29:PRO:HB3	38:BG:160:ALA:HB2	2.03	0.41
37:BF:6:LEU:H	37:BF:16:ASP:HA	1.85	0.41
45:BP:7:VAL:HG21	45:BP:93:TRP:CH2	2.56	0.41
4:AD:25:GLU:C	4:AD:27:GLU:H	2.23	0.41
33:BA:161:A:H2'	33:BA:162:A:C8	2.55	0.41
47:BR:26:ALA:C	47:BR:28:ARG:H	2.23	0.41
43:BN:62:ILE:HA	43:BN:84:CYS:SG	2.61	0.41
25:B1:5:GLU:O	25:B1:60:ARG:NH2	2.53	0.41
28:B4:50:ASN:N	28:B4:51:GLY:HA2	2.36	0.41
31:B7:12:LYS:NZ	33:BA:252:C:O2	2.53	0.41
33:BA:1441:U:O2'	33:BA:1568:G:O2'	2.38	0.41
33:BA:16:G:H2'	33:BA:17:G:H8	1.85	0.41
1:AA:1169:G:HO2'	1:AA:1170:C:H6	1.66	0.41
33:BA:2371:C:O2'	33:BA:2403:C:H5''	2.21	0.41
33:BA:525:A:N6	33:BA:546:G:O2'	2.52	0.41
36:BE:17:ALA:O	36:BE:19:ASN:N	2.54	0.41
5:AE:46:VAL:O	5:AE:72:ILE:N	2.49	0.41
33:BA:2066:A:H2'	33:BA:2067:G:C8	2.56	0.41
1:AA:1414:G:H2'	1:AA:1415:U:C6	2.55	0.41
24:B0:38:ILE:C	24:B0:39:LEU:HD12	2.41	0.41
35:BD:246:PRO:HG3	35:BD:255:LEU:HD12	2.03	0.41
33:BA:1847:U:H4'	33:BA:1850:A:H1'	2.02	0.41
33:BA:2488:A:N6	33:BA:2523:G:N3	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:45:G:N7	33:BA:218:G:O2'	2.43	0.41
33:BA:2719:A:C2	46:BQ:17:LEU:HD11	2.55	0.41
33:BA:2144:G:O6	33:BA:2146:A:H3'	2.21	0.41
33:BA:970:A:H2'	33:BA:971:A:H8	1.84	0.41
33:BA:659:A:N1	37:BF:46:GLN:HG3	2.36	0.41
33:BA:661:A:H2'	33:BA:662:U:O4'	2.20	0.41
1:AA:266:A:H2'	1:AA:267:G:H8	1.86	0.41
1:AA:1423:C:H2'	1:AA:1424:G:H8	1.85	0.41
33:BA:983:U:H2'	33:BA:984:G:C8	2.56	0.41
33:BA:984:G:H2'	33:BA:985:G:H8	1.85	0.41
1:AA:1084:G:H1	1:AA:1093:U:H3	1.68	0.41
1:AA:36:C:H2'	1:AA:37:G:C8	2.56	0.41
33:BA:726:C:H2'	33:BA:727:A:C8	2.56	0.41
31:B7:42:ARG:NH2	33:BA:2378:G:OP2	2.54	0.41
1:AA:1380:G:O3'	9:AI:71:GLY:HA3	2.21	0.41
33:BA:2593:A:OP1	33:BA:2677:G:O2'	2.26	0.41
33:BA:2623:C:N4	33:BA:2624:G:O6	2.54	0.41
33:BA:343:A:OP2	53:BX:80:ARG:NH2	2.45	0.41
50:BU:67:ARG:HD2	50:BU:89:ARG:HB2	2.02	0.41
50:BU:67:ARG:CA	50:BU:90:GLN:O	2.67	0.41
33:BA:621:G:H5'	33:BA:2531:G:C6	2.56	0.41
33:BA:620:U:O2'	33:BA:2531:G:O6	2.37	0.41
52:BW:56:ILE:CG2	52:BW:77:ARG:HE	2.33	0.41
22:AY:8:G:C3'	22:AY:9:A:C8	3.00	0.41
33:BA:2613:U:H3'	33:BA:2614:U:H5'	2.01	0.41
33:BA:837:U:O2'	33:BA:838:C:P	2.78	0.41
33:BA:1586:G:O2'	33:BA:1587:U:O4'	2.29	0.41
33:BA:1600:G:N2	33:BA:1600:G:OP2	2.30	0.41
1:AA:1522:U:H2'	1:AA:1523:A:C8	2.56	0.41
33:BA:1013:U:H2'	33:BA:1014:A:C8	2.56	0.41
1:AA:988:A:N6	1:AA:1327:A:H62	2.19	0.41
1:AA:1495:U:H2'	1:AA:1496:G:C8	2.55	0.41
33:BA:1029:A:N6	33:BA:1030:G:O6	2.51	0.41
38:BG:111:VAL:HB	38:BG:114:PHE:HB3	2.02	0.41
1:AA:738:A:N6	1:AA:739:G:C6	2.89	0.41
33:BA:340:U:H5''	53:BX:83:TYR:HB2	2.02	0.41
33:BA:167:U:H2'	33:BA:168:A:C8	2.55	0.41
53:BX:64:HIS:HD2	53:BX:66:SER:OG	2.03	0.41
33:BA:2393:C:H2'	33:BA:2394:G:O4'	2.21	0.41
52:BW:91:GLU:HG3	52:BW:92:ILE:HG13	2.03	0.41
28:B4:6:ARG:NH2	33:BA:2048:U:H3'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:669:C:OP2	44:BO:104:LYS:NZ	2.40	0.41
47:BR:82:ALA:O	47:BR:86:ALA:N	2.54	0.41
1:AA:792:C:H2'	1:AA:793:A:H8	1.86	0.41
1:AA:792:C:H2'	1:AA:793:A:C8	2.56	0.41
33:BA:2725:U:H2'	33:BA:2726:G:C8	2.56	0.41
44:BO:46:VAL:HG22	44:BO:47:ARG:H	1.86	0.41
1:AA:245:C:H2'	1:AA:246:G:C8	2.55	0.41
1:AA:151:A:H3'	1:AA:152:C:H6	1.86	0.41
1:AA:248:C:HO2'	1:AA:249:G:H8	1.65	0.41
1:AA:1513:A:H5'	1:AA:1541:A:O4'	2.20	0.41
1:AA:390:A:H2'	1:AA:391:A:H8	1.85	0.41
33:BA:1831:A:HO2'	33:BA:1832:A:H8	1.65	0.41
1:AA:590:G:N1	1:AA:768:A:OP2	2.38	0.41
33:BA:2237:C:H2'	33:BA:2238:C:C6	2.56	0.41
24:B0:37:ARG:HH11	24:B0:44:PRO:CB	2.29	0.41
24:B0:37:ARG:CD	24:B0:45:LYS:HD3	2.47	0.41
37:BF:126:LEU:O	37:BF:195:THR:HA	2.22	0.41
39:BH:4:VAL:HG13	39:BH:70:ARG:HH21	1.86	0.41
33:BA:2878:U:H2'	33:BA:2879:G:C8	2.56	0.41
33:BA:2188:G:H2'	33:BA:2189:G:C8	2.56	0.41
33:BA:365:U:N3	33:BA:385:G:O2'	2.41	0.41
33:BA:1820:A:H4'	35:BD:205:ILE:HB	2.03	0.41
23:AZ:80:MET:HG3	23:AZ:81:ASN:N	2.35	0.41
33:BA:726:C:H2'	33:BA:727:A:H8	1.86	0.41
51:BV:66:ALA:HA	51:BV:69:LEU:HD12	2.03	0.41
33:BA:1060:U:H2'	33:BA:1061:A:H8	1.85	0.41
33:BA:892:U:O2'	33:BA:893:A:H5'	2.20	0.41
1:AA:363:C:H1'	1:AA:396:G:H1'	2.02	0.41
1:AA:335:A:O2'	1:AA:336:C:O4'	2.37	0.41
33:BA:1823:U:H2'	33:BA:1824:C:C6	2.55	0.41
33:BA:1378:G:H5'	52:BW:16:ARG:HG3	2.02	0.41
33:BA:847:A:H1'	33:BA:849:A:OP2	2.21	0.41
38:BG:102:LYS:NZ	38:BG:140:GLU:OE2	2.41	0.41
37:BF:65:TRP:CZ2	37:BF:75:GLN:HG3	2.56	0.40
30:B6:1:MET:CG	33:BA:800:G:OP1	2.69	0.40
33:BA:1657:C:C5'	33:BA:1657:C:H6	2.34	0.40
43:BN:22:ILE:HD11	43:BN:42:THR:HG23	2.03	0.40
51:BV:8:ARG:HA	51:BV:102:HIS:CD2	2.56	0.40
46:BQ:78:ASP:OD1	46:BQ:79:ALA:N	2.53	0.40
48:BS:61:THR:HG22	48:BS:78:PRO:HA	2.02	0.40
33:BA:2334:U:N3	38:BG:151:GLY:HA3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:2863:G:H1	33:BA:2905:C:H42	1.67	0.40
33:BA:1006:A:O5'	33:BA:1006:A:H8	2.04	0.40
44:BO:47:ARG:HA	44:BO:48:PRO:HD3	1.95	0.40
35:BD:208:ALA:O	35:BD:211:SER:OG	2.30	0.40
36:BE:14:GLN:HB3	36:BE:22:LEU:HD11	2.03	0.40
33:BA:1596:U:H2'	33:BA:1597:C:C6	2.56	0.40
50:BU:78:PRO:O	50:BU:79:LYS:HB2	2.21	0.40
22:AY:14:G:O2'	22:AY:15:A:C2	2.58	0.40
33:BA:1474:C:H42	33:BA:1618:A:N6	2.11	0.40
33:BA:2568:C:H2'	33:BA:2569:C:H5''	2.03	0.40
44:BO:23:ILE:HG23	50:BU:81:ASN:O	2.20	0.40
33:BA:1304:G:H2'	33:BA:2043:A:N6	2.36	0.40
33:BA:2070:U:H2'	33:BA:2071:A:C8	2.56	0.40
38:BG:33:LYS:HD3	38:BG:92:ARG:NH1	2.36	0.40
46:BQ:17:LEU:HD21	46:BQ:39:GLU:OE1	2.21	0.40
1:AA:495:U:H2'	1:AA:496:A:C8	2.56	0.40
33:BA:852:G:H5'	33:BA:853:C:C5	2.56	0.40
33:BA:1247:G:O2'	33:BA:1248:C:H6	2.05	0.40
33:BA:2468:A:H5'	33:BA:2468:A:C8	2.56	0.40
33:BA:2868:G:H2'	33:BA:2869:A:C8	2.56	0.40
1:AA:468:C:H2'	1:AA:469:G:H8	1.87	0.40
33:BA:1825:U:H2'	33:BA:1826:C:C6	2.55	0.40
48:BS:25:PRO:HG3	48:BS:53:ARG:HG3	2.03	0.40
1:AA:1129:U:H3	1:AA:1163:G:H1	1.68	0.40
33:BA:1396:C:H2'	33:BA:1397:G:O4'	2.22	0.40
33:BA:865:G:H21	33:BA:1230:A:H62	1.68	0.40
33:BA:1251:U:O2	33:BA:1251:U:C2'	2.69	0.40
35:BD:231:PRO:HB2	35:BD:243:ARG:NH2	2.36	0.40
33:BA:1660:C:O2'	33:BA:1661:A:H3'	2.22	0.40
1:AA:268:G:N2	1:AA:273:G:C6	2.89	0.40
1:AA:1332:G:H2'	1:AA:1333:A:C8	2.56	0.40
33:BA:1756:U:H2'	33:BA:1757:G:C2	2.57	0.40
33:BA:275:A:N6	33:BA:296:G:N2	2.69	0.40
33:BA:675:C:O2	33:BA:685:U:O2'	2.34	0.40
1:AA:848:G:H2'	1:AA:849:G:H8	1.86	0.40
33:BA:31:C:O2'	33:BA:1278:G:OP1	2.35	0.40
33:BA:1153:G:OP1	40:BJ:59:MET:HG2	2.21	0.40
39:BH:76:MET:O	39:BH:80:VAL:HG23	2.21	0.40
1:AA:1418:C:N4	1:AA:1419:A:H62	2.19	0.40
38:BG:13:ALA:O	38:BG:17:MET:HG2	2.22	0.40
33:BA:2010:A:N3	33:BA:2010:A:C2'	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BA:721:G:H1'	37:BF:74:ARG:CD	2.51	0.40
37:BF:126:LEU:HD21	37:BF:146:LEU:HD11	2.03	0.40
28:B4:41:ARG:HG2	46:BQ:103:LYS:HB3	2.03	0.40
33:BA:1562:A:H3'	33:BA:1563:G:C8	2.55	0.40
51:BV:8:ARG:O	51:BV:10:VAL:N	2.50	0.40
1:AA:988:A:C6	1:AA:1327:A:N6	2.89	0.40
26:B2:22:THR:HG22	33:BA:897:G:O2'	2.20	0.40
33:BA:2405:A:H2'	33:BA:2406:A:O4'	2.21	0.40
33:BA:2566:U:H2'	33:BA:2567:C:C6	2.56	0.40
33:BA:1087:U:H2'	33:BA:1088:G:H8	1.86	0.40
21:AX:47:U:H4'	21:AX:48:C:H5'	2.04	0.40
1:AA:932:G:H2'	1:AA:933:A:C8	2.56	0.40
33:BA:1867:C:H4'	33:BA:1868:G:C8	2.56	0.40
45:BP:65:TRP:HB2	45:BP:105:GLU:HB2	2.03	0.40
25:B1:49:ALA:HA	25:B1:52:ARG:HG2	2.04	0.40
33:BA:2468:A:O2'	33:BA:2469:C:OP2	2.33	0.40
37:BF:49:HIS:CD2	37:BF:92:PRO:HB2	2.56	0.40
31:B7:2:PRO:N	33:BA:635:C:H1'	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/246 (90%)	204 (92%)	13 (6%)	5 (2%)	8	50
3	AC	208/218 (95%)	193 (93%)	14 (7%)	1 (0%)	34	76
4	AD	197/200 (98%)	191 (97%)	4 (2%)	2 (1%)	19	64
5	AE	163/166 (98%)	150 (92%)	9 (6%)	4 (2%)	7	48
6	AF	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	8	50
7	AG	151/156 (97%)	144 (95%)	6 (4%)	1 (1%)	26	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	129/132 (98%)	123 (95%)	5 (4%)	1 (1%)	24	68
9	AI	128/130 (98%)	113 (88%)	10 (8%)	5 (4%)	4	37
10	AJ	100/102 (98%)	88 (88%)	8 (8%)	4 (4%)	4	37
11	AK	116/131 (88%)	106 (91%)	9 (8%)	1 (1%)	21	65
12	AL	135/138 (98%)	119 (88%)	9 (7%)	7 (5%)	2	31
13	AM	117/121 (97%)	94 (80%)	13 (11%)	10 (8%)	1	17
14	AN	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	31
15	AO	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	8	50
16	AP	87/90 (97%)	82 (94%)	3 (3%)	2 (2%)	8	50
17	AQ	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
18	AR	69/79 (87%)	64 (93%)	2 (3%)	3 (4%)	3	35
19	AS	82/92 (89%)	75 (92%)	5 (6%)	2 (2%)	7	49
20	AT	84/88 (96%)	77 (92%)	6 (7%)	1 (1%)	16	61
23	AZ	22/95 (23%)	17 (77%)	2 (9%)	3 (14%)	0	6
24	B0	56/62 (90%)	53 (95%)	1 (2%)	2 (4%)	4	40
25	B1	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
26	B2	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	11	54
27	B3	62/66 (94%)	56 (90%)	4 (6%)	2 (3%)	5	43
28	B4	52/59 (88%)	47 (90%)	4 (8%)	1 (2%)	10	53
29	B5	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	B6	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
31	B7	62/66 (94%)	56 (90%)	5 (8%)	1 (2%)	12	56
32	B8	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
35	BD	273/277 (99%)	264 (97%)	8 (3%)	1 (0%)	39	79
36	BE	205/209 (98%)	189 (92%)	11 (5%)	5 (2%)	7	49
37	BF	203/207 (98%)	184 (91%)	16 (8%)	3 (2%)	13	57
38	BG	176/179 (98%)	154 (88%)	18 (10%)	4 (2%)	8	50
39	BH	173/179 (97%)	165 (95%)	7 (4%)	1 (1%)	30	73
40	BJ	121/166 (73%)	97 (80%)	14 (12%)	10 (8%)	1	18
41	BK	131/141 (93%)	122 (93%)	7 (5%)	2 (2%)	13	57
42	BM	140/145 (97%)	130 (93%)	9 (6%)	1 (1%)	26	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BN	120/122 (98%)	112 (93%)	6 (5%)	2 (2%)	11	55
44	BO	144/146 (99%)	132 (92%)	10 (7%)	2 (1%)	14	58
45	BP	136/144 (94%)	129 (95%)	7 (5%)	0	100	100
46	BQ	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	21	65
47	BR	118/120 (98%)	106 (90%)	7 (6%)	5 (4%)	3	35
48	BS	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
49	BT	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
50	BU	99/102 (97%)	82 (83%)	15 (15%)	2 (2%)	9	52
51	BV	107/113 (95%)	96 (90%)	8 (8%)	3 (3%)	6	46
52	BW	91/95 (96%)	86 (94%)	5 (6%)	0	100	100
53	BX	98/103 (95%)	87 (89%)	8 (8%)	3 (3%)	5	44
54	BZ	80/94 (85%)	77 (96%)	3 (4%)	0	100	100
All	All	5563/5920 (94%)	5116 (92%)	336 (6%)	111 (2%)	14	52

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	4	ILE
6	AF	70	ALA
12	AL	127	ARG
13	AM	101	ASN
23	AZ	78	PHE
23	AZ	84	VAL
40	BJ	93	ALA
41	BK	19	ASN
47	BR	26	ALA
53	BX	87	ASP
2	AB	18	HIS
2	AB	36	ASN
2	AB	104	PHE
5	AE	163	GLU
6	AF	54	ASP
7	AG	54	THR
8	AH	71	GLU
9	AI	106	ARG
9	AI	122	ARG
12	AL	38	VAL
13	AM	41	GLU

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Mol	Chain	Res	Type
13	AM	46	ARG
13	AM	65	VAL
13	AM	102	SER
13	AM	112	PRO
27	B3	49	PHE
36	BE	18	GLU
36	BE	78	ARG
36	BE	90	ALA
36	BE	99	VAL
38	BG	42	ASP
40	BJ	48	ALA
40	BJ	72	LEU
40	BJ	89	VAL
40	BJ	108	ILE
40	BJ	124	LYS
47	BR	68	THR
47	BR	91	SER
51	BV	8	ARG
3	AC	60	ALA
4	AD	5	THR
9	AI	57	THR
10	AJ	35	SER
12	AL	32	LYS
12	AL	39	SER
12	AL	115	LEU
13	AM	42	ASP
13	AM	66	GLU
15	AO	88	ARG
19	AS	84	ALA
23	AZ	77	VAL
31	B7	31	HIS
37	BF	4	VAL
40	BJ	55	TYR
40	BJ	90	VAL
40	BJ	113	ILE
43	BN	89	ASP
47	BR	63	LEU
50	BU	28	GLU
51	BV	41	ARG
51	BV	65	ASP
53	BX	74	LYS
53	BX	89	LYS

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Mol	Chain	Res	Type
2	AB	37	GLY
4	AD	142	ARG
10	AJ	44	THR
12	AL	25	ASN
13	AM	10	PRO
16	AP	44	ALA
16	AP	47	ALA
18	AR	28	TYR
26	B2	29	LYS
28	B4	45	ALA
35	BD	245	SER
36	BE	54	ASP
37	BF	128	ASP
38	BG	112	ARG
38	BG	147	THR
39	BH	13	SER
43	BN	34	ASN
47	BR	71	THR
10	AJ	36	VAL
12	AL	16	VAL
14	AN	31	HIS
14	AN	56	VAL
18	AR	16	CYS
19	AS	30	VAL
24	B0	44	PRO
27	B3	60	ASN
37	BF	89	VAL
40	BJ	107	GLU
42	BM	22	ALA
44	BO	107	ALA
46	BQ	110	ASP
50	BU	52	THR
5	AE	162	GLU
9	AI	104	LEU
9	AI	107	ASP
11	AK	120	HIS
20	AT	69	LYS
24	B0	40	VAL
5	AE	109	GLY
13	AM	84	GLY
14	AN	51	GLY
44	BO	88	GLY

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Mol	Chain	Res	Type
10	AJ	80	THR
15	AO	24	SER
18	AR	23	ILE
2	AB	201	PRO
38	BG	25	VAL
41	BK	24	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AZ	6/87 (7%)	4 (67%)	2 (33%)	0	3
24	B0	47/50 (94%)	47 (100%)	0	100	100
25	B1	56/57 (98%)	56 (100%)	0	100	100
26	B2	52/53 (98%)	52 (100%)	0	100	100
27	B3	53/55 (96%)	53 (100%)	0	100	100
28	B4	48/53 (91%)	48 (100%)	0	100	100
29	B5	46/47 (98%)	46 (100%)	0	100	100
30	B6	39/39 (100%)	39 (100%)	0	100	100
31	B7	54/56 (96%)	54 (100%)	0	100	100
32	B8	34/35 (97%)	34 (100%)	0	100	100
35	BD	223/225 (99%)	223 (100%)	0	100	100
36	BE	168/170 (99%)	168 (100%)	0	100	100
37	BF	169/170 (99%)	168 (99%)	1 (1%)	90	95
38	BG	153/154 (99%)	153 (100%)	0	100	100
39	BH	148/151 (98%)	148 (100%)	0	100	100
40	BJ	105/138 (76%)	105 (100%)	0	100	100
41	BK	103/110 (94%)	103 (100%)	0	100	100
42	BM	120/123 (98%)	120 (100%)	0	100	100
43	BN	101/101 (100%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BO	110/110 (100%)	110 (100%)	0	100	100
45	BP	111/116 (96%)	111 (100%)	0	100	100
46	BQ	99/100 (99%)	99 (100%)	0	100	100
47	BR	93/93 (100%)	93 (100%)	0	100	100
48	BS	99/100 (99%)	99 (100%)	0	100	100
49	BT	96/98 (98%)	96 (100%)	0	100	100
50	BU	83/84 (99%)	83 (100%)	0	100	100
51	BV	90/93 (97%)	89 (99%)	1 (1%)	80	90
52	BW	84/85 (99%)	84 (100%)	0	100	100
53	BX	84/87 (97%)	84 (100%)	0	100	100
54	BZ	64/74 (86%)	64 (100%)	0	100	100
All	All	2738/2914 (94%)	2734 (100%)	4 (0%)	95	97

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

Mol	Chain	Res	Type
23	AZ	81	ASN
23	AZ	86	ASP
37	BF	66	ARG
51	BV	90	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
24	B0	23	ASN
26	B2	37	HIS
27	B3	20	ASN
27	B3	60	ASN
28	B4	40	HIS
29	B5	25	ASN
31	B7	35	ASN
31	B7	60	GLN
35	BD	194	GLN
35	BD	199	GLN
35	BD	264	ASN
36	BE	50	GLN
36	BE	152	ASN

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Mol	Chain	Res	Type
36	BE	172	GLN
36	BE	191	ASN
37	BF	29	ASN
37	BF	67	GLN
37	BF	75	GLN
37	BF	82	GLN
38	BG	37	ASN
39	BH	62	HIS
39	BH	107	ASN
41	BK	93	ASN
42	BM	59	ASN
44	BO	78	ASN
46	BQ	27	ASN
48	BS	15	GLN
48	BS	80	HIS
49	BT	37	GLN
49	BT	91	ASN
50	BU	65	GLN
51	BV	60	HIS
51	BV	102	HIS
53	BX	2	HIS
53	BX	39	ASN
53	BX	64	HIS
54	BZ	37	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1543/1555 (99%)	235 (15%)	17 (1%)
21	AX	76/77 (98%)	15 (19%)	1 (1%)
22	AY	18/19 (94%)	14 (77%)	3 (16%)
33	BA	2922/2928 (99%)	791 (27%)	80 (2%)
34	BB	111/119 (93%)	32 (28%)	4 (3%)
All	All	4670/4698 (99%)	1087 (23%)	105 (2%)

All (1087) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	A
1	AA	11	G
1	AA	34	A

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Mol	Chain	Res	Type
1	AA	41	G
1	AA	49	C
1	AA	50	C
1	AA	52	A
1	AA	53	A
1	AA	83	C
1	AA	85	U
1	AA	87	C
1	AA	88	U
1	AA	99	A
1	AA	114	A
1	AA	118	A
1	AA	119	C
1	AA	120	A
1	AA	127	U
1	AA	129	A
1	AA	130	C
1	AA	140	A
1	AA	142	A
1	AA	143	C
1	AA	151	A
1	AA	158	G
1	AA	162	C
1	AA	163	C
1	AA	182	U
1	AA	183	U
1	AA	194	C
1	AA	195	A
1	AA	197	G
1	AA	210	A
1	AA	222	G
1	AA	249	G
1	AA	255	G
1	AA	258	A
1	AA	259	G
1	AA	274	G
1	AA	275	C
1	AA	287	A
1	AA	288	C
1	AA	297	G
1	AA	336	C
1	AA	337	A

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Mol	Chain	Res	Type
1	AA	338	C
1	AA	340	G
1	AA	355	G
1	AA	360	C
1	AA	362	G
1	AA	375	U
1	AA	380	C
1	AA	405	A
1	AA	414	G
1	AA	419	A
1	AA	420	U
1	AA	421	G
1	AA	422	A
1	AA	429	U
1	AA	430	C
1	AA	432	G
1	AA	437	U
1	AA	456	A
1	AA	457	A
1	AA	460	A
1	AA	472	C
1	AA	474	A
1	AA	475	A
1	AA	476	U
1	AA	477	A
1	AA	488	U
1	AA	490	G
1	AA	491	A
1	AA	494	G
1	AA	506	A
1	AA	507	A
1	AA	518	A
1	AA	520	C
1	AA	527	C
1	AA	528	C
1	AA	533	G
1	AA	536	G
1	AA	541	A
1	AA	556	A
1	AA	568	A
1	AA	572	A
1	AA	581	A

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Mol	Chain	Res	Type
1	AA	582	A
1	AA	585	G
1	AA	586	G
1	AA	605	A
1	AA	642	U
1	AA	643	C
1	AA	651	A
1	AA	662	U
1	AA	674	A
1	AA	696	A
1	AA	704	A
1	AA	711	A
1	AA	727	A
1	AA	728	C
1	AA	729	C
1	AA	730	A
1	AA	732	U
1	AA	740	G
1	AA	741	C
1	AA	756	U
1	AA	757	A
1	AA	764	G
1	AA	786	A
1	AA	793	A
1	AA	802	U
1	AA	803	A
1	AA	823	A
1	AA	824	A
1	AA	826	C
1	AA	830	G
1	AA	837	A
1	AA	838	A
1	AA	843	U
1	AA	849	G
1	AA	856	C
1	AA	865	G
1	AA	874	A
1	AA	880	U
1	AA	881	U
1	AA	882	A
1	AA	883	A
1	AA	924	A

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Mol	Chain	Res	Type
1	AA	936	G
1	AA	944	C
1	AA	945	A
1	AA	948	A
1	AA	970	U
1	AA	974	A
1	AA	979	A
1	AA	981	G
1	AA	984	A
1	AA	985	A
1	AA	986	G
1	AA	987	A
1	AA	992	U
1	AA	993	A
1	AA	1003	G
1	AA	1004	A
1	AA	1012	U
1	AA	1014	A
1	AA	1018	U
1	AA	1027	U
1	AA	1028	A
1	AA	1033	G
1	AA	1036	C
1	AA	1040	U
1	AA	1042	G
1	AA	1044	G
1	AA	1046	G
1	AA	1053	G
1	AA	1054	A
1	AA	1060	G
1	AA	1064	C
1	AA	1075	U
1	AA	1104	G
1	AA	1105	U
1	AA	1111	A
1	AA	1112	A
1	AA	1143	A
1	AA	1148	G
1	AA	1149	U
1	AA	1150	U
1	AA	1151	G
1	AA	1155	A

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Mol	Chain	Res	Type
1	AA	1161	A
1	AA	1168	U
1	AA	1169	G
1	AA	1170	C
1	AA	1177	C
1	AA	1191	G
1	AA	1192	U
1	AA	1193	G
1	AA	1200	A
1	AA	1205	A
1	AA	1206	A
1	AA	1210	A
1	AA	1211	U
1	AA	1221	U
1	AA	1222	A
1	AA	1223	U
1	AA	1230	G
1	AA	1237	C
1	AA	1247	A
1	AA	1250	G
1	AA	1266	A
1	AA	1269	G
1	AA	1289	A
1	AA	1295	C
1	AA	1296	A
1	AA	1308	A
1	AA	1313	G
1	AA	1314	G
1	AA	1326	C
1	AA	1329	C
1	AA	1331	C
1	AA	1332	G
1	AA	1341	A
1	AA	1343	G
1	AA	1345	U
1	AA	1346	G
1	AA	1355	A
1	AA	1373	U
1	AA	1377	G
1	AA	1407	A
1	AA	1435	A
1	AA	1451	A

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Mol	Chain	Res	Type
1	AA	1452	G
1	AA	1455	A
1	AA	1461	U
1	AA	1462	U
1	AA	1463	A
1	AA	1464	G
1	AA	1490	A
1	AA	1502	A
1	AA	1503	A
1	AA	1504	G
1	AA	1509	A
1	AA	1513	A
1	AA	1515	G
1	AA	1516	U
1	AA	1527	G
1	AA	1539	G
1	AA	1540	G
1	AA	1541	A
1	AA	1544	A
1	AA	1545	C
1	AA	1547	U
1	AA	1548	C
21	AX	9	A
21	AX	18	G
21	AX	19	U
21	AX	21	A
21	AX	34	G
21	AX	35	U
21	AX	36	C
21	AX	48	C
21	AX	49	G
21	AX	55	U
21	AX	56	C
21	AX	57	G
21	AX	70	A
21	AX	73	G
21	AX	76	A
22	AY	2	G
22	AY	3	U
22	AY	4	G
22	AY	5	A
22	AY	6	A

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Mol	Chain	Res	Type
22	AY	7	C
22	AY	8	G
22	AY	9	A
22	AY	11	G
22	AY	12	A
22	AY	13	G
22	AY	14	G
22	AY	16	A
22	AY	17	G
33	BA	8	U
33	BA	9	U
33	BA	10	A
33	BA	13	A
33	BA	27	G
33	BA	28	A
33	BA	31	C
33	BA	34	U
33	BA	35	G
33	BA	38	A
33	BA	44	A
33	BA	45	G
33	BA	46	C
33	BA	48	G
33	BA	49	A
33	BA	51	G
33	BA	55	G
33	BA	59	G
33	BA	60	G
33	BA	61	A
33	BA	63	G
33	BA	70	G
33	BA	71	A
33	BA	75	G
33	BA	76	C
33	BA	84	A
33	BA	87	U
33	BA	90	A
33	BA	91	A
33	BA	94	A
33	BA	101	G
33	BA	102	A
33	BA	109	G

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Mol	Chain	Res	Type
33	BA	118	A
33	BA	119	U
33	BA	124	A
33	BA	125	A
33	BA	126	A
33	BA	127	C
33	BA	130	A
33	BA	133	A
33	BA	156	A
33	BA	161	A
33	BA	162	A
33	BA	163	U
33	BA	164	U
33	BA	176	A
33	BA	177	G
33	BA	179	A
33	BA	183	A
33	BA	184	G
33	BA	185	A
33	BA	188	C
33	BA	199	A
33	BA	202	A
33	BA	203	U
33	BA	207	A
33	BA	208	G
33	BA	215	G
33	BA	216	A
33	BA	217	G
33	BA	218	G
33	BA	219	A
33	BA	225	A
33	BA	226	A
33	BA	227	G
33	BA	230	A
33	BA	231	A
33	BA	232	U
33	BA	233	G
33	BA	236	A
33	BA	245	G
33	BA	248	G
33	BA	251	G
33	BA	252	C

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Mol	Chain	Res	Type
33	BA	253	G
33	BA	258	A
33	BA	267	C
33	BA	268	A
33	BA	272	C
33	BA	275	A
33	BA	282	G
33	BA	283	G
33	BA	289	C
33	BA	290	U
33	BA	291	C
33	BA	299	U
33	BA	300	G
33	BA	301	U
33	BA	302	A
33	BA	310	C
33	BA	312	G
33	BA	313	U
33	BA	314	A
33	BA	315	C
33	BA	321	U
33	BA	322	A
33	BA	324	A
33	BA	326	A
33	BA	327	G
33	BA	328	G
33	BA	337	A
33	BA	338	G
33	BA	345	A
33	BA	346	G
33	BA	349	C
33	BA	354	A
33	BA	355	A
33	BA	360	C
33	BA	367	G
33	BA	368	G
33	BA	373	A
33	BA	375	C
33	BA	376	A
33	BA	378	C
33	BA	379	C
33	BA	380	C

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Mol	Chain	Res	Type
33	BA	387	C
33	BA	390	A
33	BA	393	U
33	BA	394	U
33	BA	405	U
33	BA	406	G
33	BA	407	A
33	BA	411	G
33	BA	418	A
33	BA	419	G
33	BA	420	U
33	BA	430	C
33	BA	433	G
33	BA	434	U
33	BA	435	G
33	BA	438	A
33	BA	453	G
33	BA	459	A
33	BA	474	U
33	BA	478	U
33	BA	481	U
33	BA	485	U
33	BA	489	G
33	BA	490	A
33	BA	494	A
33	BA	502	C
33	BA	503	C
33	BA	504	A
33	BA	525	A
33	BA	526	A
33	BA	527	A
33	BA	528	G
33	BA	537	A
33	BA	538	A
33	BA	544	G
33	BA	548	A
33	BA	550	G
33	BA	551	A
33	BA	553	A
33	BA	555	C
33	BA	556	C
33	BA	558	G

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Mol	Chain	Res	Type
33	BA	559	A
33	BA	561	A
33	BA	562	C
33	BA	564	G
33	BA	575	A
33	BA	576	G
33	BA	577	U
33	BA	578	A
33	BA	589	G
33	BA	591	U
33	BA	592	A
33	BA	594	C
33	BA	595	G
33	BA	599	G
33	BA	606	U
33	BA	607	G
33	BA	616	A
33	BA	618	A
33	BA	619	A
33	BA	634	A
33	BA	637	A
33	BA	647	A
33	BA	648	G
33	BA	649	G
33	BA	650	U
33	BA	651	U
33	BA	655	C
33	BA	656	A
33	BA	657	G
33	BA	658	A
33	BA	660	G
33	BA	663	G
33	BA	664	C
33	BA	665	G
33	BA	666	G
33	BA	667	A
33	BA	668	G
33	BA	673	A
33	BA	674	G
33	BA	684	G
33	BA	691	U
33	BA	692	A

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Mol	Chain	Res	Type
33	BA	698	C
33	BA	700	U
33	BA	711	U
33	BA	718	C
33	BA	732	A
33	BA	733	U
33	BA	734	C
33	BA	736	A
33	BA	746	A
33	BA	764	C
33	BA	769	A
33	BA	774	A
33	BA	775	G
33	BA	777	C
33	BA	785	C
33	BA	786	A
33	BA	787	C
33	BA	788	G
33	BA	794	U
33	BA	795	G
33	BA	799	A
33	BA	811	A
33	BA	812	G
33	BA	822	G
33	BA	823	G
33	BA	829	A
33	BA	830	A
33	BA	831	U
33	BA	832	G
33	BA	836	A
33	BA	837	U
33	BA	838	C
33	BA	840	A
33	BA	841	A
33	BA	843	C
33	BA	847	A
33	BA	848	G
33	BA	851	A
33	BA	852	G
33	BA	853	C
33	BA	858	U
33	BA	859	C

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Mol	Chain	Res	Type
33	BA	866	A
33	BA	872	C
33	BA	874	U
33	BA	875	U
33	BA	878	G
33	BA	880	C
33	BA	882	A
33	BA	892	U
33	BA	893	A
33	BA	894	A
33	BA	895	G
33	BA	896	A
33	BA	900	U
33	BA	908	A
33	BA	910	A
33	BA	912	C
33	BA	913	A
33	BA	914	C
33	BA	915	U
33	BA	916	G
33	BA	918	U
33	BA	924	U
33	BA	925	A
33	BA	928	G
33	BA	931	C
33	BA	932	C
33	BA	933	C
33	BA	934	U
33	BA	935	A
33	BA	937	C
33	BA	942	U
33	BA	943	A
33	BA	944	C
33	BA	948	A
33	BA	952	A
33	BA	956	A
33	BA	957	A
33	BA	959	C
33	BA	964	A
33	BA	970	A
33	BA	972	U
33	BA	974	A

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Mol	Chain	Res	Type
33	BA	976	U
33	BA	977	U
33	BA	978	A
33	BA	981	C
33	BA	987	A
33	BA	992	G
33	BA	998	G
33	BA	1005	A
33	BA	1007	G
33	BA	1019	A
33	BA	1020	A
33	BA	1025	A
33	BA	1027	A
33	BA	1030	G
33	BA	1031	C
33	BA	1034	A
33	BA	1035	G
33	BA	1037	C
33	BA	1042	A
33	BA	1055	A
33	BA	1058	U
33	BA	1059	A
33	BA	1063	G
33	BA	1067	A
33	BA	1068	G
33	BA	1071	G
33	BA	1072	A
33	BA	1073	A
33	BA	1079	U
33	BA	1093	G
33	BA	1096	A
33	BA	1097	A
33	BA	1100	A
33	BA	1102	G
33	BA	1103	A
33	BA	1104	U
33	BA	1107	U
33	BA	1108	G
33	BA	1111	U
33	BA	1113	A
33	BA	1115	A
33	BA	1116	A

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Mol	Chain	Res	Type
33	BA	1117	G
33	BA	1118	C
33	BA	1121	C
33	BA	1122	C
33	BA	1123	A
33	BA	1124	C
33	BA	1126	A
33	BA	1128	U
33	BA	1129	U
33	BA	1130	A
33	BA	1131	A
33	BA	1134	A
33	BA	1135	G
33	BA	1136	U
33	BA	1138	C
33	BA	1139	G
33	BA	1141	A
33	BA	1145	G
33	BA	1148	C
33	BA	1150	C
33	BA	1152	G
33	BA	1158	G
33	BA	1177	G
33	BA	1178	U
33	BA	1179	A
33	BA	1181	C
33	BA	1182	G
33	BA	1188	A
33	BA	1189	A
33	BA	1194	A
33	BA	1197	A
33	BA	1201	A
33	BA	1202	A
33	BA	1209	G
33	BA	1218	U
33	BA	1219	C
33	BA	1220	G
33	BA	1222	A
33	BA	1236	G
33	BA	1244	A
33	BA	1246	G
33	BA	1247	G

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Mol	Chain	Res	Type
33	BA	1248	C
33	BA	1249	U
33	BA	1250	G
33	BA	1251	U
33	BA	1268	G
33	BA	1269	A
33	BA	1278	G
33	BA	1286	A
33	BA	1289	U
33	BA	1293	A
33	BA	1295	U
33	BA	1296	G
33	BA	1305	A
33	BA	1306	G
33	BA	1312	A
33	BA	1313	A
33	BA	1314	A
33	BA	1315	G
33	BA	1319	G
33	BA	1327	U
33	BA	1339	A
33	BA	1340	A
33	BA	1341	U
33	BA	1344	C
33	BA	1345	U
33	BA	1346	A
33	BA	1352	U
33	BA	1360	A
33	BA	1363	G
33	BA	1364	C
33	BA	1375	A
33	BA	1376	G
33	BA	1380	U
33	BA	1381	A
33	BA	1382	G
33	BA	1384	C
33	BA	1388	A
33	BA	1404	A
33	BA	1417	A
33	BA	1418	U
33	BA	1423	A
33	BA	1424	A

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Mol	Chain	Res	Type
33	BA	1426	A
33	BA	1432	A
33	BA	1433	U
33	BA	1434	A
33	BA	1435	U
33	BA	1436	U
33	BA	1439	U
33	BA	1441	U
33	BA	1442	A
33	BA	1450	C
33	BA	1456	A
33	BA	1459	U
33	BA	1460	G
33	BA	1464	A
33	BA	1473	A
33	BA	1474	C
33	BA	1495	C
33	BA	1496	G
33	BA	1497	G
33	BA	1498	U
33	BA	1499	A
33	BA	1504	A
33	BA	1507	U
33	BA	1513	U
33	BA	1516	A
33	BA	1517	A
33	BA	1519	C
33	BA	1520	A
33	BA	1521	G
33	BA	1523	U
33	BA	1524	A
33	BA	1528	U
33	BA	1529	G
33	BA	1530	G
33	BA	1536	A
33	BA	1539	C
33	BA	1543	U
33	BA	1553	A
33	BA	1555	A
33	BA	1558	C
33	BA	1561	G
33	BA	1562	A

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Mol	Chain	Res	Type
33	BA	1572	G
33	BA	1573	C
33	BA	1578	G
33	BA	1581	A
33	BA	1582	U
33	BA	1583	A
33	BA	1584	U
33	BA	1585	A
33	BA	1596	U
33	BA	1600	G
33	BA	1601	A
33	BA	1607	C
33	BA	1608	A
33	BA	1615	A
33	BA	1617	A
33	BA	1626	U
33	BA	1631	A
33	BA	1632	G
33	BA	1638	A
33	BA	1640	G
33	BA	1647	U
33	BA	1648	A
33	BA	1651	G
33	BA	1652	C
33	BA	1653	A
33	BA	1655	A
33	BA	1657	C
33	BA	1658	G
33	BA	1660	C
33	BA	1667	A
33	BA	1674	G
33	BA	1679	A
33	BA	1680	A
33	BA	1688	G
33	BA	1691	A
33	BA	1693	C
33	BA	1695	A
33	BA	1696	G
33	BA	1697	A
33	BA	1707	U
33	BA	1708	U
33	BA	1712	G

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Mol	Chain	Res	Type
33	BA	1713	A
33	BA	1719	G
33	BA	1727	A
33	BA	1728	C
33	BA	1739	C
33	BA	1744	G
33	BA	1745	A
33	BA	1752	G
33	BA	1756	U
33	BA	1757	G
33	BA	1758	U
33	BA	1759	U
33	BA	1767	A
33	BA	1769	G
33	BA	1771	C
33	BA	1774	A
33	BA	1776	A
33	BA	1777	G
33	BA	1778	A
33	BA	1780	C
33	BA	1781	C
33	BA	1782	G
33	BA	1785	G
33	BA	1787	G
33	BA	1788	A
33	BA	1790	U
33	BA	1791	A
33	BA	1792	G
33	BA	1793	G
33	BA	1796	C
33	BA	1802	A
33	BA	1810	G
33	BA	1811	C
33	BA	1814	A
33	BA	1829	C
33	BA	1830	G
33	BA	1831	A
33	BA	1832	A
33	BA	1834	C
33	BA	1839	A
33	BA	1858	A
33	BA	1862	C

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Mol	Chain	Res	Type
33	BA	1876	A
33	BA	1877	A
33	BA	1882	A
33	BA	1897	C
33	BA	1900	A
33	BA	1901	A
33	BA	1902	G
33	BA	1910	G
33	BA	1912	G
33	BA	1913	A
33	BA	1916	U
33	BA	1918	A
33	BA	1919	A
33	BA	1925	A
33	BA	1930	A
33	BA	1935	G
33	BA	1942	A
33	BA	1943	C
33	BA	1944	U
33	BA	1948	A
33	BA	1954	C
33	BA	1959	G
33	BA	1960	U
33	BA	1966	A
33	BA	1967	A
33	BA	1968	U
33	BA	1969	U
33	BA	1972	U
33	BA	1981	A
33	BA	1984	U
33	BA	1992	C
33	BA	1995	A
33	BA	1996	C
33	BA	1999	A
33	BA	2000	A
33	BA	2001	G
33	BA	2010	A
33	BA	2011	U
33	BA	2012	C
33	BA	2020	U
33	BA	2024	U
33	BA	2026	A

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Mol	Chain	Res	Type
33	BA	2027	A
33	BA	2033	G
33	BA	2042	A
33	BA	2047	A
33	BA	2052	A
33	BA	2059	A
33	BA	2060	A
33	BA	2062	A
33	BA	2072	C
33	BA	2084	C
33	BA	2085	G
33	BA	2088	A
33	BA	2089	A
33	BA	2090	G
33	BA	2091	A
33	BA	2092	C
33	BA	2098	G
33	BA	2111	A
33	BA	2116	G
33	BA	2121	U
33	BA	2122	G
33	BA	2123	A
33	BA	2124	A
33	BA	2125	U
33	BA	2133	C
33	BA	2140	U
33	BA	2142	C
33	BA	2143	A
33	BA	2145	G
33	BA	2147	U
33	BA	2149	G
33	BA	2155	A
33	BA	2156	G
33	BA	2157	C
33	BA	2161	G
33	BA	2162	G
33	BA	2165	A
33	BA	2175	C
33	BA	2176	A
33	BA	2177	G
33	BA	2188	G
33	BA	2190	C

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Mol	Chain	Res	Type
33	BA	2195	G
33	BA	2197	G
33	BA	2200	A
33	BA	2202	A
33	BA	2205	A
33	BA	2214	G
33	BA	2220	A
33	BA	2222	C
33	BA	2227	A
33	BA	2232	G
33	BA	2233	C
33	BA	2240	U
33	BA	2241	A
33	BA	2243	C
33	BA	2246	G
33	BA	2252	A
33	BA	2254	A
33	BA	2255	C
33	BA	2267	G
33	BA	2268	G
33	BA	2279	G
33	BA	2295	A
33	BA	2296	A
33	BA	2308	G
33	BA	2312	C
33	BA	2315	A
33	BA	2333	G
33	BA	2334	U
33	BA	2335	U
33	BA	2336	G
33	BA	2337	G
33	BA	2339	A
33	BA	2340	A
33	BA	2343	A
33	BA	2345	U
33	BA	2346	C
33	BA	2347	G
33	BA	2348	C
33	BA	2349	A
33	BA	2350	G
33	BA	2351	A
33	BA	2352	G

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Mol	Chain	Res	Type
33	BA	2356	A
33	BA	2357	A
33	BA	2362	A
33	BA	2363	C
33	BA	2364	A
33	BA	2369	A
33	BA	2376	C
33	BA	2377	U
33	BA	2379	C
33	BA	2387	A
33	BA	2390	A
33	BA	2400	G
33	BA	2411	G
33	BA	2412	G
33	BA	2414	C
33	BA	2420	G
33	BA	2421	A
33	BA	2431	U
33	BA	2435	C
33	BA	2453	C
33	BA	2454	A
33	BA	2455	A
33	BA	2456	C
33	BA	2458	G
33	BA	2459	A
33	BA	2460	U
33	BA	2463	A
33	BA	2464	A
33	BA	2468	A
33	BA	2469	C
33	BA	2470	C
33	BA	2477	A
33	BA	2483	G
33	BA	2505	A
33	BA	2513	G
33	BA	2523	G
33	BA	2528	C
33	BA	2531	G
33	BA	2532	A
33	BA	2533	U
33	BA	2534	G
33	BA	2536	C

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Mol	Chain	Res	Type
33	BA	2541	C
33	BA	2542	A
33	BA	2543	U
33	BA	2546	C
33	BA	2547	A
33	BA	2558	G
33	BA	2569	C
33	BA	2570	A
33	BA	2571	A
33	BA	2572	G
33	BA	2575	U
33	BA	2576	U
33	BA	2583	U
33	BA	2594	A
33	BA	2595	A
33	BA	2596	G
33	BA	2601	A
33	BA	2602	C
33	BA	2610	G
33	BA	2611	G
33	BA	2614	U
33	BA	2619	A
33	BA	2630	C
33	BA	2631	A
33	BA	2638	U
33	BA	2639	C
33	BA	2642	U
33	BA	2648	U
33	BA	2658	A
33	BA	2661	A
33	BA	2663	A
33	BA	2668	A
33	BA	2680	C
33	BA	2683	A
33	BA	2684	G
33	BA	2711	G
33	BA	2714	G
33	BA	2717	G
33	BA	2718	U
33	BA	2720	C
33	BA	2730	U
33	BA	2731	G

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Mol	Chain	Res	Type
33	BA	2743	G
33	BA	2754	A
33	BA	2755	U
33	BA	2766	G
33	BA	2773	G
33	BA	2779	A
33	BA	2780	G
33	BA	2784	C
33	BA	2785	U
33	BA	2786	A
33	BA	2787	A
33	BA	2790	A
33	BA	2794	A
33	BA	2795	G
33	BA	2797	C
33	BA	2798	C
33	BA	2800	C
33	BA	2804	A
33	BA	2807	A
33	BA	2808	U
33	BA	2809	G
33	BA	2813	U
33	BA	2818	C
33	BA	2819	A
33	BA	2820	U
33	BA	2825	C
33	BA	2826	A
33	BA	2843	G
33	BA	2855	G
33	BA	2858	U
33	BA	2859	G
33	BA	2860	A
33	BA	2869	A
33	BA	2873	G
33	BA	2874	G
33	BA	2892	G
33	BA	2897	G
33	BA	2898	A
33	BA	2899	C
33	BA	2902	A
33	BA	2905	C
33	BA	2909	U

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Mol	Chain	Res	Type
33	BA	2918	G
33	BA	2919	A
34	BB	10	G
34	BB	11	A
34	BB	12	U
34	BB	13	A
34	BB	20	A
34	BB	23	U
34	BB	28	C
34	BB	37	A
34	BB	39	A
34	BB	40	C
34	BB	41	C
34	BB	42	G
34	BB	46	A
34	BB	48	G
34	BB	49	G
34	BB	50	A
34	BB	51	A
34	BB	55	A
34	BB	59	U
34	BB	60	C
34	BB	61	U
34	BB	63	C
34	BB	64	A
34	BB	81	G
34	BB	85	U
34	BB	86	U
34	BB	87	U
34	BB	88	C
34	BB	96	G
34	BB	97	A
34	BB	107	G
34	BB	110	G

All (105) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	98	U
1	AA	113	G
1	AA	119	C
1	AA	126	G

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Mol	Chain	Res	Type
1	AA	436	G
1	AA	641	G
1	AA	842	U
1	AA	848	G
1	AA	855	G
1	AA	864	U
1	AA	873	U
1	AA	1111	A
1	AA	1154	C
1	AA	1210	A
1	AA	1461	U
1	AA	1501	G
1	AA	1544	A
21	AX	47	U
22	AY	10	U
22	AY	12	A
22	AY	13	G
33	BA	43	G
33	BA	58	G
33	BA	90	A
33	BA	118	A
33	BA	124	A
33	BA	163	U
33	BA	175	G
33	BA	183	A
33	BA	207	A
33	BA	229	A
33	BA	252	C
33	BA	271	C
33	BA	288	C
33	BA	298	U
33	BA	366	A
33	BA	377	G
33	BA	405	U
33	BA	419	G
33	BA	526	A
33	BA	549	A
33	BA	647	A
33	BA	649	G
33	BA	666	G
33	BA	683	A
33	BA	717	A

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Mol	Chain	Res	Type
33	BA	785	C
33	BA	837	U
33	BA	847	A
33	BA	934	U
33	BA	936	C
33	BA	1019	A
33	BA	1066	A
33	BA	1092	A
33	BA	1103	A
33	BA	1107	U
33	BA	1117	G
33	BA	1173	A
33	BA	1245	G
33	BA	1250	G
33	BA	1305	A
33	BA	1339	A
33	BA	1351	U
33	BA	1434	A
33	BA	1438	C
33	BA	1455	C
33	BA	1527	C
33	BA	1535	U
33	BA	1581	A
33	BA	1595	U
33	BA	1630	G
33	BA	1652	C
33	BA	1679	A
33	BA	1755	C
33	BA	1779	G
33	BA	1784	A
33	BA	1813	A
33	BA	1876	A
33	BA	1965	A
33	BA	2155	A
33	BA	2187	A
33	BA	2254	A
33	BA	2267	G
33	BA	2278	U
33	BA	2295	A
33	BA	2334	U
33	BA	2348	C
33	BA	2351	A

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Mol	Chain	Res	Type
33	BA	2454	A
33	BA	2468	A
33	BA	2504	C
33	BA	2595	A
33	BA	2631	A
33	BA	2683	A
33	BA	2710	C
33	BA	2716	U
33	BA	2779	A
33	BA	2784	C
33	BA	2785	U
33	BA	2807	A
33	BA	2812	A
34	BB	38	U
34	BB	47	C
34	BB	54	U
34	BB	59	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.