



Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 03:16 pm BST

PDB ID : 9SD9 / pdb_00009sd9
EMDB ID : EMD-54779
Title : 6-Helix Bundle - with a Clasp (6HB-C)-dimer with 2'-Fluoro-modified pyrimidines (FY RNA)
Authors : Kristoffersen, E.L.; Andersen, E.S.; Zwergius, N.H.
Deposited on : 2025-08-12
Resolution : 9.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

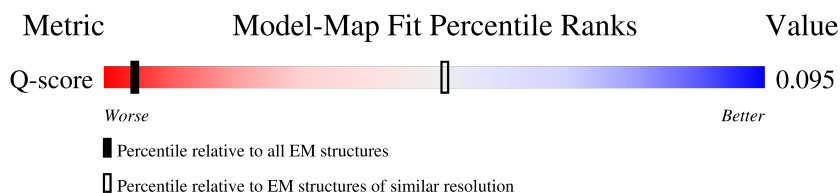
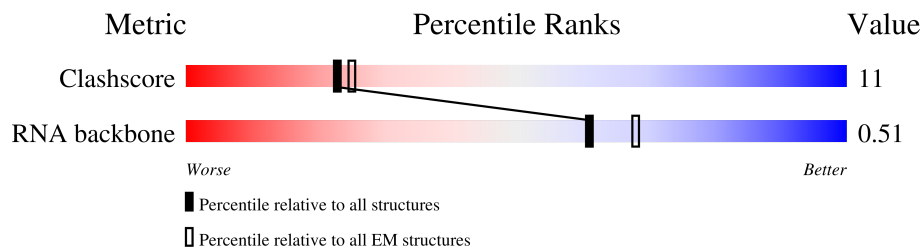
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

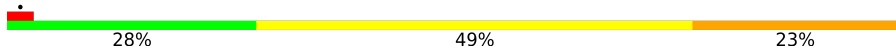
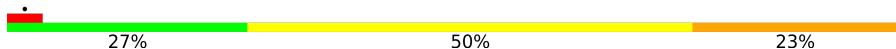
The reported resolution of this entry is 9.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
RNA backbone	8273	3508	-
Q-score	-	25397	185 (9.10 - 10.10)

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

Mol	Chain	Length	Quality of chain
1	A	720	
1	B	720	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	UFT	B	720	X	-	-	-

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30671 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.

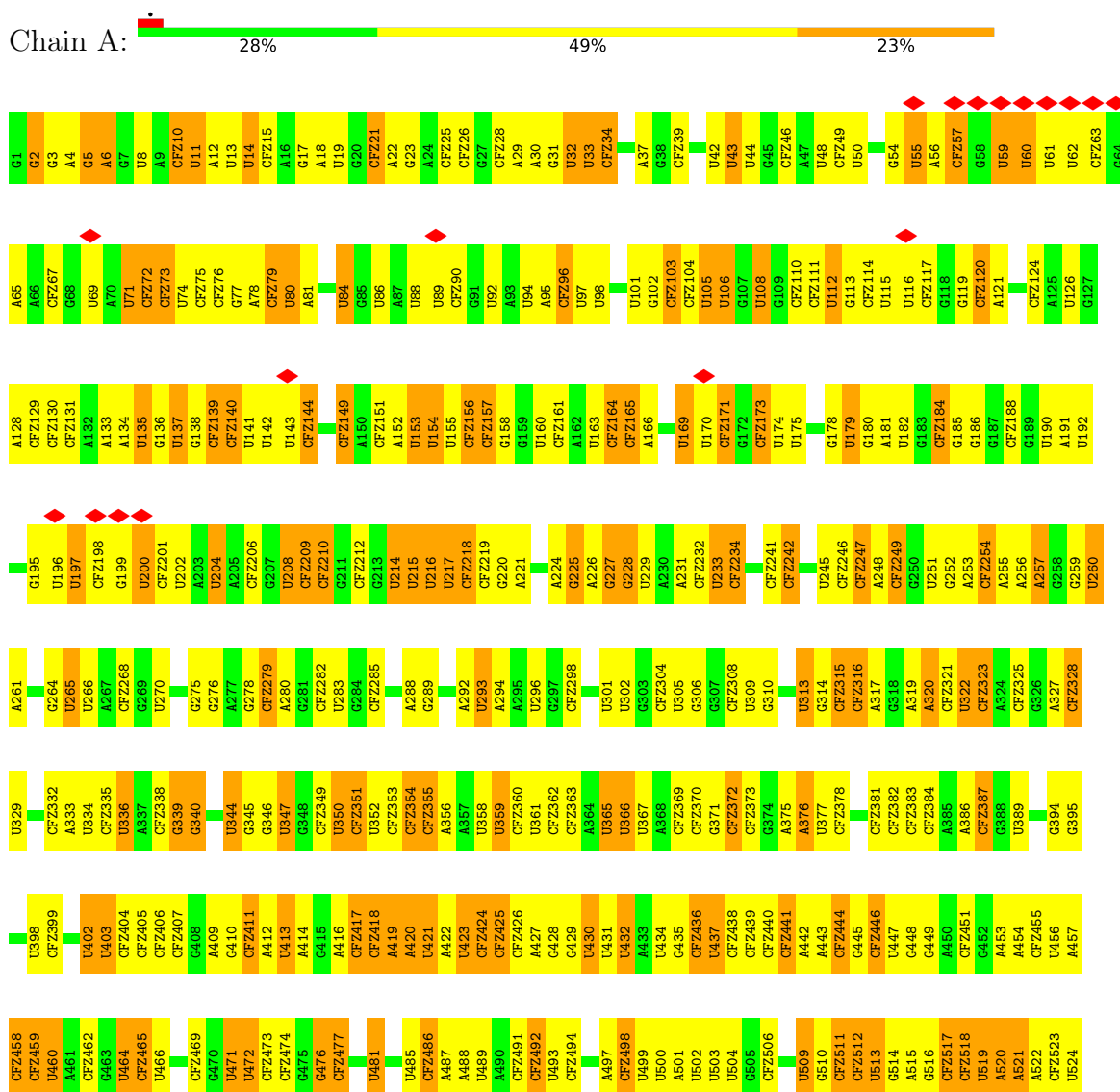
- Molecule 1 is a RNA chain called RNA (720-MER).

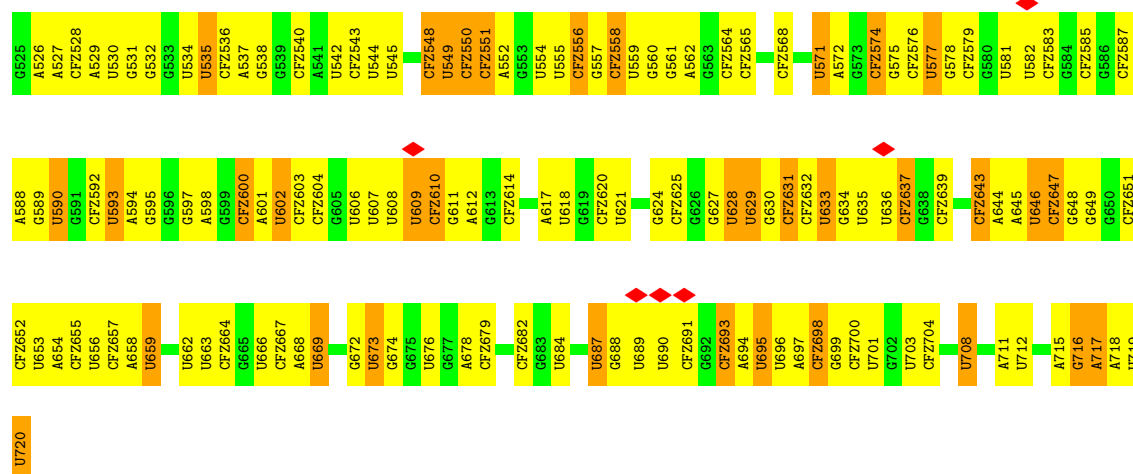
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	F	N	O	P		
1	A	720	15334	6843	357	2708	4707	719	0	0
1	B	720	15337	6843	357	2708	4709	720	0	0

3 Residue-property plots

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

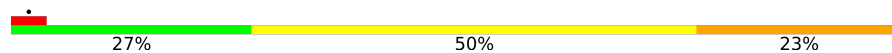
• Molecule 1: RNA (720-MER)





• Molecule 1: RNA (720-MER)

Chain B:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.650	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.128	Depositor
Map size (\AA)	465.8432, 465.8432, 465.8432	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.8197, 1.8197, 1.8197	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UFT, CFZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	6/9186 (0.1%)	0.26	2/14187 (0.0%)
1	B	0.47	5/9189 (0.1%)	0.24	0/14191
All	All	0.47	11/18375 (0.1%)	0.25	2/28378 (0.0%)

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	B	1	0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	UFT	O3'-P	5.40	1.61	1.56
1	B	389	UFT	O3'-P	5.08	1.61	1.56
1	A	101	UFT	O3'-P	5.07	1.61	1.56
1	A	684	UFT	O3'-P	5.04	1.61	1.56
1	B	432	UFT	O3'-P	5.03	1.61	1.56
1	B	296	UFT	O3'-P	5.02	1.61	1.56
1	A	524	UFT	O3'-P	5.02	1.61	1.56
1	B	50	UFT	O3'-P	5.01	1.61	1.56
1	A	293	UFT	O3'-P	5.01	1.61	1.56
1	A	44	UFT	O3'-P	5.01	1.61	1.56
1	B	530	UFT	O3'-P	5.00	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	A	OP1-P-O3'	-8.91	81.27	108.00
1	A	520	A	OP2-P-O3'	-7.93	84.20	108.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	720	UFT	C2'

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15334	0	7387	225	0
1	B	15337	0	7384	236	0
All	All	30671	0	14771	458	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 11.

All (458) 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)
1:A:225:G:H1	1:B:494:CFZ:HN4	1.19	0.87
1:A:481:UFT:HN3	1:A:501:A:H61	1.24	0.84
1:B:481:UFT:HN3	1:B:501:A:H61	1.25	0.83
1:B:135:UFT:HN3	1:B:152:A:H61	1.27	0.81
1:B:602:UFT:HN3	1:B:617:A:H61	1.30	0.78
1:A:602:UFT:HN3	1:A:617:A:H61	1.31	0.76
1:B:659:UFT:HN3	1:B:668:A:H61	1.33	0.75
1:B:629:UFT:H2'	1:B:630:G:H8	1.53	0.74
1:A:629:UFT:H2'	1:A:630:G:H8	1.53	0.73
1:A:658:A:H61	1:A:669:UFT:HN3	1.34	0.73
1:A:54:G:H1	1:A:71:UFT:HN3	1.37	0.72
1:A:135:UFT:HN3	1:A:152:A:H61	1.38	0.71
1:A:293:UFT:HN3	1:A:422:A:H61	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:UFT:HN3	1:B:422:A:H61	1.36	0.70
1:A:279:CFZ:H2'	1:A:280:A:H8	1.57	0.70
1:B:279:CFZ:H2'	1:B:280:A:H8	1.57	0.69
1:A:84:UFT:HN3	1:A:95:A:H61	1.42	0.68
1:A:376:A:H61	1:A:402:UFT:HN3	1.39	0.68
1:B:376:A:H61	1:B:402:UFT:HN3	1.39	0.68
1:B:246:CFZ:H2'	1:B:247:CFZ:H6	1.76	0.68
1:B:442:A:H61	1:B:472:UFT:HN3	1.41	0.67
1:A:227:G:H1	1:B:492:CFZ:HN4	1.43	0.66
1:B:33:UFT:H2'	1:B:34:CFZ:H6	1.77	0.66
1:A:659:UFT:HN3	1:A:668:A:H61	1.43	0.66
1:B:550:CFZ:H2'	1:B:551:CFZ:H6	1.78	0.65
1:B:385:A:H61	1:B:393:A:H61	1.44	0.65
1:A:492:CFZ:N4	1:B:228:G:O6	2.29	0.65
1:B:227:G:H2'	1:B:228:G:H8	1.63	0.63
1:A:12:A:N6	1:A:345:G:O6	2.32	0.62
1:B:577:UFT:H2'	1:B:578:G:H8	1.65	0.62
1:A:513:UFT:HN3	1:A:537:A:H61	1.45	0.62
1:B:32:UFT:H2'	1:B:33:UFT:H6	1.82	0.62
1:A:442:A:H61	1:A:472:UFT:HN3	1.46	0.61
1:B:436:CFZ:H2'	1:B:437:UFT:H6	1.82	0.61
1:B:492:CFZ:O5'	1:B:492:CFZ:H6	2.00	0.61
1:B:2:G:H3'	1:B:3:G:H5''	1.81	0.61
1:A:521:A:H61	1:A:529:A:H61	1.48	0.61
1:A:275:G:N2	1:A:276:G:O6	2.34	0.60
1:A:436:CFZ:H2'	1:A:437:UFT:H6	1.82	0.60
1:B:153:UFT:H2'	1:B:154:UFT:H6	1.83	0.60
1:B:319:A:N6	1:B:328:CFZ:O2	2.34	0.60
1:A:134:A:H2'	1:A:135:UFT:H6	1.83	0.60
1:A:153:UFT:H2'	1:A:154:UFT:H6	1.82	0.60
1:B:134:A:H2'	1:B:135:UFT:H6	1.83	0.60
1:B:275:G:N2	1:B:276:G:O6	2.33	0.60
1:B:678:A:H2'	1:B:679:CFZ:H6	1.84	0.60
1:A:313:UFT:HN3	1:A:333:A:H61	1.49	0.60
1:A:515:A:H2	1:A:535:UFT:HN3	1.50	0.60
1:B:549:UFT:H2'	1:B:550:CFZ:H6	1.83	0.59
1:A:120:CFZ:H2'	1:A:121:A:H8	1.67	0.59
1:B:135:UFT:H2'	1:B:136:G:C8	2.38	0.59
1:B:120:CFZ:H2'	1:B:121:A:H8	1.67	0.59
1:B:365:UFT:H2'	1:B:366:UFT:H6	1.85	0.59
1:B:217:UFT:H2'	1:B:218:CFZ:H6	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:A:H61	1:A:593:UFT:HN3	1.51	0.58
1:A:577:UFT:HN3	1:A:588:A:H61	1.52	0.58
1:A:693:CFZ:H2'	1:A:694:A:H8	1.69	0.58
1:B:600:CFZ:H2'	1:B:601:A:H8	1.68	0.58
1:B:247:CFZ:H2'	1:B:248:A:H8	1.69	0.58
1:A:135:UFT:H2'	1:A:136:G:C8	2.39	0.58
1:A:497:A:H2'	1:A:498:CFZ:H5	1.84	0.57
1:A:257:A:H61	1:A:460:UFT:HN3	1.53	0.57
1:B:257:A:H61	1:B:460:UFT:HN3	1.52	0.57
1:B:179:UFT:H2'	1:B:180:G:C8	2.40	0.57
1:B:247:CFZ:H2'	1:B:248:A:C8	2.40	0.57
1:B:472:UFT:H5'	1:B:594:A:H5''	1.87	0.57
1:A:179:UFT:H2'	1:A:180:G:C8	2.40	0.56
1:B:513:UFT:HN3	1:B:537:A:H61	1.52	0.56
1:A:316:CFZ:H2'	1:A:317:A:C8	2.41	0.56
1:B:693:CFZ:H2'	1:B:694:A:H8	1.69	0.56
1:B:84:UFT:HN3	1:B:95:A:H61	1.51	0.56
1:A:112:UFT:H2'	1:A:113:G:C8	2.40	0.56
1:B:112:UFT:H2'	1:B:113:G:C8	2.41	0.56
1:B:316:CFZ:H2'	1:B:317:A:C8	2.41	0.56
1:B:362:CFZ:F2'	1:B:363:CFZ:O4'	2.14	0.56
1:B:490:A:H2'	1:B:491:CFZ:H6	1.87	0.56
1:A:217:UFT:H2'	1:A:218:CFZ:H6	1.87	0.56
1:B:492:CFZ:C4	1:B:493:UFT:H5	2.36	0.56
1:B:551:CFZ:H2'	1:B:552:A:C8	2.41	0.55
1:B:279:CFZ:H2'	1:B:280:A:C8	2.41	0.55
1:A:316:CFZ:H2'	1:A:317:A:H8	1.71	0.55
1:B:560:G:H2'	1:B:561:G:H8	1.72	0.55
1:A:411:CFZ:H2'	1:A:412:A:H8	1.72	0.55
1:A:548:CFZ:H2'	1:A:549:UFT:H6	1.88	0.55
1:B:509:UFT:H2'	1:B:510:G:H8	1.72	0.55
1:B:629:UFT:H2'	1:B:630:G:C8	2.40	0.55
1:B:21:CFZ:H2'	1:B:22:A:C8	2.43	0.54
1:B:519:UFT:HN3	1:B:531:G:H1	1.56	0.54
1:B:647:CFZ:H2'	1:B:648:G:C8	2.43	0.54
1:B:179:UFT:H2'	1:B:180:G:H8	1.73	0.54
1:B:411:CFZ:H2'	1:B:412:A:H8	1.73	0.54
1:B:577:UFT:H2'	1:B:578:G:C8	2.43	0.54
1:A:509:UFT:H2'	1:A:510:G:H8	1.73	0.54
1:A:600:CFZ:H2'	1:A:601:A:H8	1.72	0.54
1:A:698:CFZ:H2'	1:A:699:G:H8	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:UFT:H2'	1:A:366:UFT:H6	1.90	0.54
1:B:21:CFZ:H2'	1:B:22:A:H8	1.73	0.54
1:B:715:A:H2'	1:B:716:G:C8	2.43	0.53
1:A:80:UFT:H2'	1:A:81:A:H8	1.74	0.53
1:A:339:G:O2'	1:A:340:G:OP1	2.23	0.53
1:A:294:A:H61	1:A:421:UFT:HN3	1.57	0.53
1:A:414:A:H2	1:A:432:UFT:HN3	1.55	0.53
1:A:179:UFT:H2'	1:A:180:G:H8	1.73	0.53
1:A:647:CFZ:H2'	1:A:648:G:C8	2.43	0.53
1:B:216:UFT:H2'	1:B:217:UFT:H6	1.90	0.53
1:B:357:A:N6	1:B:719:UFT:O4	2.42	0.53
1:A:551:CFZ:H2'	1:A:552:A:C8	2.44	0.53
1:B:548:CFZ:H2'	1:B:549:UFT:H6	1.89	0.53
1:B:698:CFZ:H2'	1:B:699:G:H8	1.74	0.53
1:A:279:CFZ:H2'	1:A:280:A:C8	2.41	0.53
1:A:556:CFZ:F2'	1:A:557:G:O4'	2.17	0.53
1:A:394:G:H2'	1:A:395:G:H8	1.75	0.53
1:B:1:G:O4'	1:B:720:UFT:F2'	2.17	0.52
1:A:55:UFT:H2'	1:A:56:A:C8	2.44	0.52
1:A:21:CFZ:H2'	1:A:22:A:C8	2.44	0.52
1:A:80:UFT:H2'	1:A:81:A:C8	2.45	0.52
1:A:5:G:N2	1:A:351:CFZ:O2	2.37	0.52
1:A:33:UFT:H2'	1:A:34:CFZ:H6	1.92	0.52
1:B:441:CFZ:H2'	1:B:442:A:C8	2.45	0.51
1:A:344:UFT:H5'A	1:A:344:UFT:H6	1.92	0.51
1:A:356:A:H61	1:A:720:UFT:HN3	1.58	0.51
1:A:600:CFZ:H2'	1:A:601:A:C8	2.45	0.51
1:B:658:A:H61	1:B:669:UFT:HN3	1.57	0.51
1:A:78:A:H2'	1:A:79:CFZ:H6	1.93	0.51
1:B:497:A:H2'	1:B:498:CFZ:H5	1.92	0.51
1:A:214:UFT:H2'	1:A:215:UFT:H6	1.92	0.51
1:A:577:UFT:H2'	1:A:578:G:H8	1.76	0.51
1:B:294:A:H61	1:B:421:UFT:HN3	1.58	0.51
1:B:137:UFT:H2'	1:B:138:G:H8	1.76	0.51
1:B:389:UFT:H2'	1:B:390:G:H8	1.76	0.50
1:A:157:CFZ:H2'	1:A:158:G:C8	2.47	0.50
1:A:355:CFZ:H2'	1:A:356:A:C8	2.46	0.50
1:A:11:UFT:H2'	1:A:12:A:C8	2.46	0.50
1:B:120:CFZ:H2'	1:B:121:A:C8	2.45	0.50
1:B:509:UFT:H2'	1:B:510:G:C8	2.46	0.50
1:A:247:CFZ:H2'	1:A:248:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:CFZ:H2'	1:B:317:A:H8	1.75	0.50
1:A:102:G:O2'	1:A:339:G:OP1	2.29	0.50
1:A:514:G:H2'	1:A:515:A:C8	2.47	0.50
1:A:645:A:H2'	1:A:646:UFT:H6	1.93	0.50
1:B:525:G:H2'	1:B:526:A:H8	1.77	0.50
1:A:509:UFT:H2'	1:A:510:G:C8	2.46	0.50
1:B:95:A:H2'	1:B:96:CFZ:H6	1.94	0.50
1:B:515:A:H2	1:B:535:UFT:HN3	1.59	0.50
1:B:670:G:H2'	1:B:671:A:H8	1.76	0.50
1:B:627:G:H1	1:B:646:UFT:HN3	1.60	0.50
1:A:199:G:H1'	1:A:200:UFT:H5	1.93	0.49
1:B:600:CFZ:H2'	1:B:601:A:C8	2.44	0.49
1:A:216:UFT:H2'	1:A:217:UFT:H6	1.93	0.49
1:A:354:CFZ:H2'	1:A:355:CFZ:H6	1.94	0.49
1:B:558:CFZ:H6	1:B:558:CFZ:O5'	2.13	0.49
1:A:165:CFZ:H2'	1:A:166:A:H8	1.77	0.49
1:A:365:UFT:HN3	1:A:711:A:H61	1.60	0.49
1:A:139:CFZ:H2'	1:A:140:CFZ:H6	1.94	0.49
1:A:157:CFZ:H2'	1:A:158:G:H8	1.78	0.49
1:B:165:CFZ:H2'	1:B:166:A:H8	1.78	0.49
1:B:444:CFZ:H2'	1:B:445:G:H8	1.78	0.49
1:A:59:UFT:H2'	1:A:60:UFT:H6	1.93	0.49
1:A:184:CFZ:H2'	1:A:185:G:C8	2.48	0.49
1:A:254:CFZ:O2P	1:A:255:A:O2'	2.29	0.49
1:A:458:CFZ:H2'	1:A:459:CFZ:H6	1.95	0.49
1:A:260:UFT:HN3	1:A:457:A:H61	1.61	0.49
1:B:128:A:O2'	1:B:306:G:O4'	2.27	0.49
1:B:633:UFT:H2'	1:B:634:G:C8	2.48	0.49
1:B:645:A:H2'	1:B:646:UFT:H6	1.93	0.49
1:B:28:CFZ:HN4	1:B:37:A:H61	1.59	0.49
1:B:139:CFZ:H2'	1:B:140:CFZ:H6	1.93	0.49
1:B:184:CFZ:H2'	1:B:185:G:C8	2.48	0.49
1:B:514:G:N2	1:B:536:CFZ:O2	2.45	0.49
1:A:629:UFT:H2'	1:A:630:G:C8	2.41	0.49
1:B:51:A:H61	1:B:74:UFT:HN3	1.59	0.49
1:B:413:UFT:H2'	1:B:414:A:C8	2.48	0.49
1:A:137:UFT:H2'	1:A:138:G:H8	1.78	0.49
1:B:222:G:H3'	1:B:223:A:H2'	1.94	0.49
1:B:510:G:H2'	1:B:511:CFZ:H6	1.95	0.49
1:A:510:G:H2'	1:A:511:CFZ:H6	1.95	0.48
1:B:8:UFT:H2'	1:B:9:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:CFZ:F2'	1:B:557:G:O4'	2.21	0.48
1:A:633:UFT:H2'	1:A:634:G:C8	2.48	0.48
1:B:157:CFZ:H2'	1:B:158:G:C8	2.48	0.48
1:A:191:A:H61	1:A:204:UFT:HN3	1.60	0.48
1:A:476:G:H3'	1:A:477:CFZ:H5'	1.96	0.48
1:A:120:CFZ:H2'	1:A:121:A:C8	2.46	0.48
1:A:252:G:H2'	1:A:253:A:C8	2.49	0.48
1:B:476:G:H3'	1:B:477:CFZ:H5'	1.96	0.48
1:A:443:A:H61	1:A:471:UFT:C4	2.26	0.48
1:A:446:CFZ:H6	1:A:446:CFZ:O5'	2.14	0.48
1:A:574:CFZ:H6	1:A:574:CFZ:O5'	2.14	0.48
1:A:654:A:N6	1:A:674:G:O6	2.47	0.48
1:B:157:CFZ:H2'	1:B:158:G:H8	1.78	0.48
1:B:719:UFT:H3'	1:B:720:UFT:H5'A	1.96	0.48
1:A:444:CFZ:H2'	1:A:445:G:H8	1.79	0.48
1:B:80:UFT:H2'	1:B:81:A:C8	2.49	0.48
1:B:718:A:H2'	1:B:719:UFT:C6	2.44	0.47
1:A:322:UFT:H2'	1:A:323:CFZ:H6	1.96	0.47
1:B:55:UFT:H2'	1:B:56:A:C8	2.49	0.47
1:B:260:UFT:HN3	1:B:457:A:H61	1.62	0.47
1:B:292:A:H61	1:B:423:UFT:HN3	1.61	0.47
1:B:252:G:H2'	1:B:253:A:C8	2.50	0.47
1:B:389:UFT:H2'	1:B:390:G:C8	2.49	0.47
1:B:418:CFZ:H3'	1:B:419:A:H2'	1.97	0.47
1:A:21:CFZ:H2'	1:A:22:A:H8	1.77	0.47
1:A:173:CFZ:H6	1:A:173:CFZ:O5'	2.15	0.47
1:A:344:UFT:H2'	1:A:345:G:C8	2.50	0.47
1:B:551:CFZ:H2'	1:B:552:A:H8	1.78	0.47
1:A:516:G:H2'	1:A:517:CFZ:H6	1.96	0.47
1:A:549:UFT:H2'	1:A:550:CFZ:H6	1.96	0.47
1:B:54:G:H1	1:B:71:UFT:HN3	1.63	0.47
1:B:314:G:H2'	1:B:315:CFZ:C6	2.44	0.47
1:B:357:A:N6	1:B:720:UFT:O2	2.48	0.47
1:B:458:CFZ:H2'	1:B:459:CFZ:H6	1.97	0.47
1:A:77:G:H2'	1:A:78:A:H8	1.80	0.47
1:A:128:A:O2'	1:A:306:G:O4'	2.27	0.47
1:A:135:UFT:H2'	1:A:136:G:H8	1.80	0.47
1:A:165:CFZ:H2'	1:A:166:A:C8	2.50	0.47
1:A:327:A:H3'	1:A:328:CFZ:H5'	1.97	0.47
1:A:716:G:O2'	1:A:717:A:OP1	2.29	0.47
1:B:601:A:H2'	1:B:602:UFT:H6	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:G:H2'	1:B:613:G:N3	2.29	0.47
1:B:486:CFZ:H2'	1:B:487:A:C8	2.49	0.47
1:A:519:UFT:HN3	1:A:531:G:H1	1.63	0.47
1:A:413:UFT:H2'	1:A:414:A:C8	2.50	0.46
1:B:246:CFZ:H2'	1:B:247:CFZ:C6	2.44	0.46
1:B:710:G:H2'	1:B:711:A:C8	2.50	0.46
1:A:419:A:H4'	1:A:420:A:O5'	2.15	0.46
1:A:2:G:H1	1:A:354:CFZ:HN4	1.63	0.46
1:A:5:G:O2'	1:A:6:A:OP1	2.27	0.46
1:B:55:UFT:HN3	1:B:70:A:H61	1.61	0.46
1:B:135:UFT:H2'	1:B:136:G:H8	1.78	0.46
1:B:531:G:H21	1:B:555:UFT:HN3	1.62	0.46
1:B:226:A:H2'	1:B:227:G:C8	2.51	0.46
1:A:292:A:H61	1:A:423:UFT:HN3	1.62	0.46
1:B:28:CFZ:HN4	1:B:37:A:N6	2.14	0.46
1:B:260:UFT:H2'	1:B:261:A:H8	1.81	0.46
1:B:446:CFZ:O5'	1:B:446:CFZ:H6	2.15	0.46
1:A:643:CFZ:H6	1:A:643:CFZ:O5'	2.16	0.46
1:B:654:A:N6	1:B:674:G:O6	2.49	0.46
1:A:669:UFT:H6	1:A:669:UFT:O5'	2.16	0.46
1:B:414:A:H2	1:B:432:UFT:HN3	1.62	0.46
1:A:561:G:H2'	1:A:562:A:H8	1.81	0.45
1:A:672:G:H2'	1:A:673:UFT:H6	1.97	0.45
1:B:341:G:N2	1:B:342:G:N7	2.56	0.45
1:B:409:A:H2'	1:B:410:G:C8	2.51	0.45
1:B:419:A:H4'	1:B:420:A:O5'	2.15	0.45
1:B:672:G:H2'	1:B:673:UFT:H6	1.98	0.45
1:A:411:CFZ:H2'	1:A:412:A:C8	2.51	0.45
1:A:486:CFZ:H2'	1:A:487:A:C8	2.52	0.45
1:B:220:G:H2'	1:B:221:A:H8	1.82	0.45
1:B:375:A:H61	1:B:403:UFT:HN3	1.63	0.45
1:A:260:UFT:H2'	1:A:261:A:H8	1.81	0.45
1:A:441:CFZ:H2'	1:A:442:A:C8	2.52	0.45
1:B:24:A:O2'	1:B:25:CFZ:O1P	2.35	0.45
1:A:5:G:H2'	1:A:6:A:C8	2.52	0.45
1:A:375:A:H61	1:A:403:UFT:HN3	1.64	0.45
1:A:418:CFZ:H3'	1:A:419:A:H2'	1.97	0.45
1:B:411:CFZ:H2'	1:B:412:A:C8	2.51	0.45
1:B:487:A:H4'	1:B:488:A:O5'	2.17	0.45
1:B:693:CFZ:H2'	1:B:694:A:C8	2.51	0.45
1:A:79:CFZ:H2'	1:A:80:UFT:H6	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:CFZ:O5'	1:A:558:CFZ:H6	2.16	0.45
1:A:597:G:H2'	1:A:598:A:H8	1.82	0.45
1:A:610:CFZ:H4'	1:A:611:G:C4	2.51	0.45
1:A:633:UFT:H2'	1:A:634:G:H8	1.82	0.45
1:B:149:CFZ:O5'	1:B:149:CFZ:H6	2.16	0.45
1:B:687:UFT:H2'	1:B:688:G:H8	1.82	0.45
1:A:409:A:H2'	1:A:410:G:C8	2.51	0.45
1:B:173:CFZ:H6	1:B:173:CFZ:O5'	2.16	0.45
1:B:429:G:H2'	1:B:430:UFT:H6	1.99	0.45
1:B:643:CFZ:O5'	1:B:643:CFZ:H6	2.17	0.45
1:A:355:CFZ:H2'	1:A:356:A:H8	1.81	0.45
1:B:5:G:H22	1:B:351:CFZ:C2	2.29	0.45
1:B:133:A:H2'	1:B:134:A:H8	1.82	0.45
1:A:10:CFZ:H2'	1:A:11:UFT:H6	1.98	0.45
1:B:13:UFT:F2'	1:B:14:UFT:O4'	2.25	0.45
1:B:327:A:H3'	1:B:328:CFZ:H5'	1.98	0.45
1:B:597:G:H2'	1:B:598:A:H8	1.82	0.45
1:B:712:UFT:H6	1:B:712:UFT:O5'	2.18	0.45
1:A:11:UFT:HN3	1:A:345:G:H1	1.64	0.44
1:A:359:UFT:HN3	1:A:717:A:H61	1.64	0.44
1:A:96:CFZ:H6	1:A:96:CFZ:O5'	2.17	0.44
1:A:694:A:H2'	1:A:695:UFT:H6	1.98	0.44
1:A:186:G:H22	1:A:209:CFZ:C2	2.31	0.44
1:A:208:UFT:H2'	1:A:209:CFZ:H6	1.99	0.44
1:A:698:CFZ:H2'	1:A:699:G:C8	2.52	0.44
1:B:338:CFZ:H6	1:B:338:CFZ:O5'	2.17	0.44
1:B:412:A:N6	1:B:435:G:O6	2.49	0.44
1:B:220:G:H2'	1:B:221:A:C8	2.52	0.44
1:B:698:CFZ:H2'	1:B:699:G:C8	2.52	0.44
1:B:715:A:H2'	1:B:716:G:H8	1.82	0.44
1:A:601:A:H2'	1:A:602:UFT:H6	1.99	0.44
1:B:204:UFT:H2'	1:B:205:A:C8	2.51	0.44
1:B:697:A:H2'	1:B:698:CFZ:H6	1.99	0.44
1:A:55:UFT:H2'	1:A:56:A:H8	1.81	0.44
1:A:133:A:H2'	1:A:134:A:H8	1.83	0.44
1:A:531:G:H2'	1:A:532:G:C8	2.53	0.44
1:A:687:UFT:H2'	1:A:688:G:C8	2.52	0.44
1:A:169:UFT:H6	1:A:169:UFT:O5'	2.18	0.44
1:A:259:G:H2'	1:A:260:UFT:H6	1.99	0.44
1:A:697:A:H2'	1:A:698:CFZ:H6	1.99	0.44
1:B:10:CFZ:HN4	1:B:346:G:H1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:G:N2	1:B:197:UFT:O4	2.51	0.44
1:B:233:UFT:H2'	1:B:234:CFZ:O4'	2.18	0.44
1:B:592:CFZ:F2'	1:B:593:UFT:OP1	2.26	0.44
1:B:694:A:H2'	1:B:695:UFT:H6	2.00	0.44
1:A:137:UFT:O5'	1:A:137:UFT:H6	2.18	0.43
1:B:209:CFZ:H2'	1:B:210:CFZ:H6	2.00	0.43
1:B:489:UFT:H2'	1:B:490:A:C8	2.53	0.43
1:B:633:UFT:H2'	1:B:634:G:H8	1.82	0.43
1:B:687:UFT:H2'	1:B:688:G:C8	2.53	0.43
1:A:149:CFZ:H6	1:A:149:CFZ:O5'	2.17	0.43
1:A:248:A:H2'	1:A:249:CFZ:H6	2.00	0.43
1:A:416:A:H61	1:A:430:UFT:HN3	1.65	0.43
1:A:549:UFT:H2'	1:A:550:CFZ:C6	2.48	0.43
1:A:687:UFT:H2'	1:A:688:G:H8	1.82	0.43
1:A:693:CFZ:H2'	1:A:694:A:C8	2.51	0.43
1:B:443:A:H61	1:B:471:UFT:C4	2.28	0.43
1:B:493:UFT:N3	1:B:494:CFZ:H5	2.33	0.43
1:A:209:CFZ:H2'	1:A:210:CFZ:H6	2.01	0.43
1:A:339:G:H2'	1:A:340:G:H8	1.83	0.43
1:B:208:UFT:H2'	1:B:209:CFZ:H6	2.00	0.43
1:B:532:G:H1'	1:B:556:CFZ:HN4	1.83	0.43
1:A:339:G:H2'	1:A:340:G:C8	2.53	0.43
1:B:186:G:H22	1:B:209:CFZ:C2	2.31	0.43
1:B:214:UFT:H2'	1:B:215:UFT:H6	2.01	0.43
1:B:9:A:H2'	1:B:10:CFZ:O4'	2.18	0.43
1:B:224:A:H62	1:B:226:A:H62	1.66	0.43
1:A:313:UFT:H2'	1:A:314:G:H8	1.84	0.43
1:A:320:A:N6	1:A:387:CFZ:HN4A	2.15	0.43
1:A:424:CFZ:H2'	1:A:425:CFZ:H6	2.01	0.43
1:B:137:UFT:H6	1:B:137:UFT:O5'	2.18	0.43
1:B:491:CFZ:H2'	1:B:492:CFZ:H6	2.01	0.43
1:B:571:UFT:C4	1:B:594:A:H61	2.31	0.43
1:B:629:UFT:HN3	1:B:644:A:H61	1.67	0.43
1:A:429:G:H2'	1:A:430:UFT:H6	2.01	0.43
1:A:549:UFT:HN3	1:A:562:A:H61	1.66	0.43
1:A:571:UFT:H2'	1:A:572:A:H8	1.84	0.43
1:B:3:G:H2'	1:B:4:A:C8	2.54	0.43
1:B:92:UFT:H2'	1:B:93:A:H8	1.83	0.43
1:A:72:CFZ:F2'	1:A:73:CFZ:O4'	2.27	0.43
1:B:586:G:H2'	1:B:587:CFZ:H6	2.01	0.43
1:A:412:A:N6	1:A:435:G:O6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:CFZ:F2'	1:A:557:G:O5'	2.27	0.43
1:A:708:UFT:H6	1:A:708:UFT:O5'	2.19	0.43
1:B:169:UFT:O5'	1:B:169:UFT:H6	2.19	0.43
1:B:264:G:H2'	1:B:265:UFT:H6	2.01	0.43
1:B:493:UFT:H2'	1:B:493:UFT:O2	2.18	0.43
1:A:217:UFT:H2'	1:A:218:CFZ:C6	2.49	0.42
1:A:314:G:H2'	1:A:315:CFZ:C6	2.50	0.42
1:B:219:CFZ:H2'	1:B:220:G:C8	2.54	0.42
1:B:630:G:H2'	1:B:631:CFZ:H6	2.01	0.42
1:A:57:CFZ:H6	1:A:57:CFZ:O5'	2.19	0.42
1:A:472:UFT:H5'	1:A:594:A:OP1	2.20	0.42
1:A:556:CFZ:F2'	1:A:557:G:N3	2.43	0.42
1:B:233:UFT:H3'	1:B:234:CFZ:H5'	1.99	0.42
1:B:259:G:H2'	1:B:260:UFT:H6	2.00	0.42
1:B:424:CFZ:H2'	1:B:425:CFZ:H6	2.01	0.42
1:B:637:CFZ:O5'	1:B:637:CFZ:H6	2.19	0.42
1:A:227:G:O2'	1:A:228:G:OP1	2.34	0.42
1:B:217:UFT:H2'	1:B:218:CFZ:C6	2.49	0.42
1:B:281:G:H22	1:B:300:G:H22	1.67	0.42
1:B:444:CFZ:H2'	1:B:445:G:C8	2.54	0.42
1:A:310:G:H1	1:A:336:UFT:HN3	1.68	0.42
1:A:497:A:O2'	1:A:498:CFZ:O1P	2.29	0.42
1:B:171:CFZ:H6	1:B:171:CFZ:O5'	2.20	0.42
1:B:219:CFZ:H2'	1:B:220:G:H8	1.84	0.42
1:B:416:A:H2'	1:B:417:CFZ:H6	2.01	0.42
1:A:233:UFT:H3'	1:A:234:CFZ:H5'	2.01	0.42
1:B:448:G:H2'	1:B:449:G:C8	2.54	0.42
1:B:627:G:H2'	1:B:628:UFT:C6	2.50	0.42
1:A:112:UFT:H2'	1:A:113:G:H8	1.84	0.42
1:A:156:CFZ:H2'	1:A:157:CFZ:H6	2.01	0.42
1:A:171:CFZ:H6	1:A:171:CFZ:O5'	2.20	0.42
1:A:418:CFZ:H2'	1:A:419:A:C8	2.54	0.42
1:A:448:G:H2'	1:A:449:G:C8	2.54	0.42
1:A:589:G:H3'	1:A:590:UFT:H5'A	2.01	0.42
1:B:550:CFZ:H2'	1:B:551:CFZ:C6	2.45	0.42
1:A:627:G:H2'	1:A:628:UFT:C6	2.50	0.42
1:B:20:G:H2'	1:B:21:CFZ:H6	2.01	0.42
1:B:427:A:C2	1:B:428:G:C8	3.08	0.42
1:B:441:CFZ:H2'	1:B:442:A:H8	1.83	0.42
1:A:560:G:H2'	1:A:561:G:H8	1.84	0.42
1:A:627:G:H1	1:A:646:UFT:HN3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:G:H2'	1:B:282:CFZ:H6	2.01	0.42
1:B:418:CFZ:H2'	1:B:419:A:C8	2.55	0.42
1:A:14:UFT:F2'	1:A:17:G:OP2	2.28	0.42
1:A:220:G:H2'	1:A:221:A:C8	2.55	0.42
1:A:551:CFZ:H2'	1:A:552:A:H8	1.82	0.42
1:A:346:G:H2'	1:A:347:UFT:O4'	2.20	0.41
1:A:511:CFZ:H2'	1:A:512:CFZ:C6	2.49	0.41
1:B:94:UFT:O5'	1:B:94:UFT:H6	2.19	0.41
1:B:669:UFT:H6	1:B:669:UFT:O5'	2.20	0.41
1:A:29:A:H61	1:A:37:A:H61	1.68	0.41
1:A:575:G:H1	1:A:590:UFT:HN3	1.67	0.41
1:A:630:G:H2'	1:A:631:CFZ:H6	2.02	0.41
1:A:637:CFZ:H6	1:A:637:CFZ:O5'	2.20	0.41
1:A:629:UFT:HN3	1:A:644:A:H61	1.69	0.41
1:B:185:G:H2'	1:B:186:G:H8	1.86	0.41
1:B:391:A:H2'	1:B:392:G:H8	1.85	0.41
1:B:416:A:H2'	1:B:417:CFZ:C6	2.49	0.41
1:A:195:G:N2	1:A:197:UFT:O4	2.53	0.41
1:A:208:UFT:H2'	1:A:209:CFZ:C6	2.50	0.41
1:A:510:G:H2'	1:A:511:CFZ:C6	2.50	0.41
1:A:518:CFZ:F2'	1:A:519:UFT:O5'	2.28	0.41
1:A:526:A:H2'	1:A:527:A:C8	2.55	0.41
1:A:105:UFT:H3'	1:A:106:UFT:H5'A	2.02	0.41
1:A:185:G:H2'	1:A:186:G:H8	1.85	0.41
1:B:323:CFZ:H2'	1:B:324:A:C8	2.55	0.41
1:A:371:G:H2'	1:A:372:CFZ:H6	2.02	0.41
1:B:236:G:N2	1:B:237:G:O6	2.53	0.41
1:B:517:CFZ:H2'	1:B:518:CFZ:C6	2.51	0.41
1:B:561:G:H2'	1:B:562:A:H8	1.86	0.41
1:B:708:UFT:O5'	1:B:708:UFT:H6	2.20	0.41
1:A:185:G:H2'	1:A:186:G:C8	2.56	0.41
1:B:105:UFT:H3'	1:B:106:UFT:H5'A	2.02	0.41
1:B:112:UFT:H2'	1:B:113:G:H8	1.86	0.41
1:B:371:G:H2'	1:B:372:CFZ:H6	2.02	0.41
1:B:484:G:H2'	1:B:485:UFT:O4'	2.20	0.41
1:A:609:UFT:H2'	1:A:611:G:C8	2.56	0.41
1:B:80:UFT:H2'	1:B:81:A:H8	1.85	0.41
1:B:165:CFZ:H6	1:B:165:CFZ:O5'	2.21	0.41
1:A:22:A:N6	1:A:43:UFT:H5	2.36	0.41
1:A:350:UFT:H2'	1:A:351:CFZ:O4'	2.21	0.41
1:B:393:A:C2	1:B:394:G:C8	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:UFT:H2'	1:B:465:CFZ:H6	2.02	0.41
1:A:264:G:H2'	1:A:265:UFT:H6	2.02	0.41
1:A:441:CFZ:H2'	1:A:442:A:H8	1.86	0.41
1:B:191:A:H61	1:B:204:UFT:HN3	1.68	0.41
1:B:720:UFT:OP1	1:B:720:UFT:H4'	2.20	0.41
1:A:32:UFT:H2'	1:A:33:UFT:H6	2.01	0.40
1:A:102:G:H2'	1:A:103:CFZ:H6	2.03	0.40
1:B:31:G:O2'	1:B:32:UFT:H6	2.21	0.40
1:B:156:CFZ:H2'	1:B:157:CFZ:H6	2.02	0.40
1:A:278:G:H2'	1:A:279:CFZ:H6	2.04	0.40
1:A:313:UFT:HN3	1:A:333:A:N6	2.18	0.40
1:A:427:A:C2	1:A:428:G:C8	3.08	0.40
1:B:53:G:H2'	1:B:54:G:H8	1.86	0.40
1:A:416:A:H2'	1:A:417:CFZ:C6	2.51	0.40
1:A:464:UFT:H2'	1:A:465:CFZ:H6	2.03	0.40
1:B:55:UFT:H2'	1:B:56:A:H8	1.87	0.40
1:B:278:G:H2'	1:B:279:CFZ:H6	2.03	0.40
1:B:511:CFZ:H2'	1:B:512:CFZ:C6	2.52	0.40
1:A:108:UFT:O5'	1:A:108:UFT:H6	2.22	0.40
1:A:144:CFZ:O5'	1:A:144:CFZ:H6	2.22	0.40
1:A:519:UFT:F2'	1:A:520:A:O5'	2.29	0.40
1:B:134:A:H2'	1:B:135:UFT:C6	2.49	0.40
1:B:185:G:H2'	1:B:186:G:C8	2.56	0.40
1:B:323:CFZ:H2'	1:B:324:A:H8	1.85	0.40
1:A:158:G:H22	1:A:242:CFZ:C2	2.33	0.40
1:A:164:CFZ:H2'	1:A:165:CFZ:C6	2.51	0.40
1:A:319:A:N6	1:A:328:CFZ:O2	2.54	0.40
1:A:411:CFZ:H6	1:A:411:CFZ:O5'	2.22	0.40
1:A:457:A:H2'	1:A:458:CFZ:H6	2.03	0.40
1:B:106:UFT:H5'A	1:B:106:UFT:H6	2.04	0.40
1:B:208:UFT:H2'	1:B:209:CFZ:C6	2.51	0.40
1:B:260:UFT:H2'	1:B:261:A:C8	2.57	0.40
1:B:372:CFZ:H6	1:B:372:CFZ:O5'	2.22	0.40
1:B:491:CFZ:H2'	1:B:492:CFZ:C6	2.52	0.40
1:B:620:CFZ:H6	1:B:620:CFZ:O5'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	185/720 (25%)	43 (23%)	6 (3%)
1	B	186/720 (25%)	41 (22%)	5 (2%)
All	All	371/1440 (25%)	84 (22%)	11 (2%)

All (84) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	G
1	A	4	A
1	A	5	G
1	A	6	A
1	A	18	A
1	A	23	G
1	A	30	A
1	A	31	G
1	A	65	A
1	A	119	G
1	A	178	G
1	A	181	A
1	A	224	A
1	A	225	G
1	A	226	A
1	A	227	G
1	A	228	G
1	A	231	A
1	A	256	A
1	A	257	A
1	A	288	A
1	A	289	G

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Mol	Chain	Res	Type
1	A	320	A
1	A	340	G
1	A	376	A
1	A	386	A
1	A	420	A
1	A	453	A
1	A	454	A
1	A	476	G
1	A	488	A
1	A	521	A
1	A	522	A
1	A	538	G
1	A	595	G
1	A	612	A
1	A	624	G
1	A	649	G
1	A	678	A
1	A	715	A
1	A	717	A
1	A	718	A
1	B	2	G
1	B	3	G
1	B	4	A
1	B	5	G
1	B	6	A
1	B	17	G
1	B	18	A
1	B	23	G
1	B	30	A
1	B	31	G
1	B	65	A
1	B	119	G
1	B	178	G
1	B	181	A
1	B	223	A
1	B	224	A
1	B	225	G
1	B	226	A
1	B	228	G
1	B	231	A
1	B	256	A
1	B	257	A

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Mol	Chain	Res	Type
1	B	288	A
1	B	289	G
1	B	340	G
1	B	341	G
1	B	376	A
1	B	420	A
1	B	453	A
1	B	454	A
1	B	476	G
1	B	488	A
1	B	496	G
1	B	521	A
1	B	522	A
1	B	538	G
1	B	595	G
1	B	612	A
1	B	624	G
1	B	649	G
1	B	678	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	3	G
1	A	5	G
1	A	227	G
1	A	339	G
1	A	419	A
1	A	716	G
1	B	5	G
1	B	227	G
1	B	230	A
1	B	419	A
1	B	487	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	B	155	1	18,21,22	2.58	9 (50%)	26,30,33	1.95	8 (30%)
1	UFT	A	530	1	18,21,22	2.64	9 (50%)	26,30,33	1.85	8 (30%)
1	UFT	A	143	1	18,21,22	2.58	9 (50%)	26,30,33	2.10	8 (30%)
1	UFT	A	200	1	18,21,22	2.54	9 (50%)	26,30,33	2.04	7 (26%)
1	CFZ	B	446	1	18,21,22	2.48	7 (38%)	26,30,33	1.43	3 (11%)
1	UFT	B	504	1	18,21,22	2.59	11 (61%)	26,30,33	1.95	8 (30%)
1	UFT	A	358	1	18,21,22	2.64	9 (50%)	26,30,33	1.84	7 (26%)
1	UFT	B	402	1	18,21,22	2.61	10 (55%)	26,30,33	1.90	7 (26%)
1	UFT	B	695	1	18,21,22	2.62	10 (55%)	26,30,33	1.90	8 (30%)
1	CFZ	B	328	1	18,21,22	2.46	7 (38%)	26,30,33	1.44	3 (11%)
1	UFT	B	42	1	18,21,22	2.68	9 (50%)	26,30,33	1.79	6 (23%)
1	UFT	A	662	1	18,21,22	2.58	9 (50%)	26,30,33	1.96	8 (30%)
1	UFT	A	542	1	18,21,22	2.59	10 (55%)	26,30,33	1.94	8 (30%)
1	CFZ	A	407	1	18,21,22	2.49	7 (38%)	26,30,33	1.24	3 (11%)
1	CFZ	B	458	1	18,21,22	2.53	7 (38%)	26,30,33	1.26	2 (7%)
1	UFT	A	115	1	18,21,22	2.57	10 (55%)	26,30,33	2.00	8 (30%)
1	CFZ	A	372	1	18,21,22	2.51	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	A	559	1	18,21,22	2.58	10 (55%)	26,30,33	1.98	7 (26%)
1	CFZ	B	540	1	18,21,22	2.52	7 (38%)	26,30,33	1.27	3 (11%)
1	CFZ	A	10	1	18,21,22	2.54	7 (38%)	26,30,33	1.15	3 (11%)
1	UFT	A	322	1	18,21,22	2.64	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	A	111	1	18,21,22	2.49	7 (38%)	26,30,33	1.37	3 (11%)
1	CFZ	B	477	1	18,21,22	2.52	7 (38%)	26,30,33	1.14	3 (11%)
1	CFZ	A	198	1	18,21,22	2.49	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	B	116	1	18,21,22	2.58	9 (50%)	26,30,33	2.07	8 (30%)
1	CFZ	A	643	1	18,21,22	2.50	7 (38%)	26,30,33	1.24	3 (11%)
1	UFT	A	233	1	18,21,22	2.59	9 (50%)	26,30,33	1.86	6 (23%)
1	CFZ	B	372	1	18,21,22	2.50	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	B	241	1	18,21,22	2.48	7 (38%)	26,30,33	1.57	4 (15%)
1	CFZ	A	438	1	18,21,22	2.48	7 (38%)	26,30,33	1.45	4 (15%)
1	UFT	A	367	1	18,21,22	2.63	9 (50%)	26,30,33	1.84	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	B	564	1	18,21,22	2.49	7 (38%)	26,30,33	1.38	2 (7%)
1	CFZ	A	462	1	18,21,22	2.50	7 (38%)	26,30,33	1.26	3 (11%)
1	UFT	A	251	1	18,21,22	2.62	10 (55%)	26,30,33	1.87	7 (26%)
1	UFT	A	636	1	18,21,22	2.57	9 (50%)	26,30,33	2.09	8 (30%)
1	UFT	B	509	1	18,21,22	2.61	10 (55%)	26,30,33	1.93	7 (26%)
1	CFZ	A	564	1	18,21,22	2.50	7 (38%)	26,30,33	1.39	2 (7%)
1	UFT	A	545	1	18,21,22	2.60	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	690	1	18,21,22	2.59	10 (55%)	26,30,33	1.90	8 (30%)
1	UFT	B	59	1	18,21,22	2.59	9 (50%)	26,30,33	2.03	7 (26%)
1	CFZ	B	558	1	18,21,22	2.49	7 (38%)	26,30,33	1.16	3 (11%)
1	CFZ	B	90	1	18,21,22	2.47	7 (38%)	26,30,33	1.50	3 (11%)
1	UFT	A	142	1	18,21,22	2.58	9 (50%)	26,30,33	2.01	8 (30%)
1	CFZ	B	219	1	18,21,22	2.53	7 (38%)	26,30,33	1.17	3 (11%)
1	UFT	A	493	1	18,21,22	2.56	9 (50%)	26,30,33	1.98	7 (26%)
1	CFZ	A	548	1	18,21,22	2.50	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	A	513	1	18,21,22	2.64	9 (50%)	26,30,33	1.82	7 (26%)
1	UFT	B	293	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	6 (23%)
1	UFT	A	42	1	18,21,22	2.64	9 (50%)	26,30,33	1.82	6 (23%)
1	UFT	B	549	1	18,21,22	2.60	9 (50%)	26,30,33	1.89	7 (26%)
1	UFT	B	719	1	18,21,22	2.59	10 (55%)	26,30,33	1.86	7 (26%)
1	UFT	B	684	1	18,21,22	2.64	9 (50%)	26,30,33	1.80	5 (19%)
1	CFZ	A	308	1	18,21,22	2.48	7 (38%)	26,30,33	1.50	4 (15%)
1	UFT	B	618	1	18,21,22	2.57	10 (55%)	26,30,33	2.04	8 (30%)
1	UFT	B	202	1	18,21,22	2.58	10 (55%)	26,30,33	2.00	8 (30%)
1	UFT	A	215	1	18,21,22	2.57	9 (50%)	26,30,33	1.97	7 (26%)
1	CFZ	B	210	1	18,21,22	2.48	7 (38%)	26,30,33	1.37	3 (11%)
1	CFZ	A	405	1	18,21,22	2.50	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	B	67	1	18,21,22	2.48	7 (38%)	26,30,33	1.39	3 (11%)
1	CFZ	A	455	1	18,21,22	2.54	7 (38%)	26,30,33	1.24	4 (15%)
1	CFZ	A	90	1	18,21,22	2.46	7 (38%)	26,30,33	1.49	3 (11%)
1	CFZ	B	164	1	18,21,22	2.50	7 (38%)	26,30,33	1.25	2 (7%)
1	CFZ	A	417	1	18,21,22	2.49	7 (38%)	26,30,33	1.46	3 (11%)
1	UFT	A	689	1	18,21,22	2.60	10 (55%)	26,30,33	1.96	7 (26%)
1	CFZ	A	25	1	18,21,22	2.49	7 (38%)	26,30,33	1.41	3 (11%)
1	CFZ	B	411	1	18,21,22	2.51	7 (38%)	26,30,33	1.20	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	B	614	1	18,21,22	2.51	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	B	485	1	18,21,22	2.58	9 (50%)	26,30,33	1.99	7 (26%)
1	UFT	A	74	1	18,21,22	2.56	10 (55%)	26,30,33	2.03	8 (30%)
1	UFT	A	635	1	18,21,22	2.59	10 (55%)	26,30,33	2.00	8 (30%)
1	UFT	B	141	1	18,21,22	2.60	9 (50%)	26,30,33	1.95	7 (26%)
1	CFZ	B	667	1	18,21,22	2.49	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	A	347	1	18,21,22	2.58	10 (55%)	26,30,33	1.89	7 (26%)
1	CFZ	B	268	1	18,21,22	2.48	7 (38%)	26,30,33	1.46	2 (7%)
1	UFT	A	366	1	18,21,22	2.58	10 (55%)	26,30,33	1.96	7 (26%)
1	UFT	B	302	1	18,21,22	2.62	9 (50%)	26,30,33	1.94	8 (30%)
1	UFT	B	94	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	8 (30%)
1	UFT	B	635	1	18,21,22	2.59	9 (50%)	26,30,33	2.00	8 (30%)
1	CFZ	B	556	1	18,21,22	2.48	7 (38%)	26,30,33	1.36	3 (11%)
1	UFT	B	365	1	18,21,22	2.61	9 (50%)	26,30,33	1.88	6 (23%)
1	UFT	B	309	1	18,21,22	2.59	9 (50%)	26,30,33	1.93	8 (30%)
1	UFT	B	313	1	18,21,22	2.60	9 (50%)	26,30,33	1.90	8 (30%)
1	CFZ	B	76	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	A	316	1	18,21,22	2.51	7 (38%)	26,30,33	1.13	2 (7%)
1	CFZ	A	79	1	18,21,22	2.51	7 (38%)	26,30,33	1.35	3 (11%)
1	CFZ	A	114	1	18,21,22	2.48	7 (38%)	26,30,33	1.44	4 (15%)
1	CFZ	B	151	1	18,21,22	2.51	7 (38%)	26,30,33	1.25	3 (11%)
1	CFZ	A	604	1	18,21,22	2.49	7 (38%)	26,30,33	1.24	4 (15%)
1	CFZ	A	165	1	18,21,22	2.52	7 (38%)	26,30,33	1.14	2 (7%)
1	UFT	A	695	1	18,21,22	2.61	9 (50%)	26,30,33	1.90	8 (30%)
1	CFZ	A	576	1	18,21,22	2.50	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	A	88	1	18,21,22	2.59	10 (55%)	26,30,33	1.93	8 (30%)
1	CFZ	B	21	1	18,21,22	2.54	7 (38%)	26,30,33	1.18	3 (11%)
1	UFT	A	633	1	18,21,22	2.61	10 (55%)	26,30,33	1.89	7 (26%)
1	CFZ	A	21	1	18,21,22	2.53	7 (38%)	26,30,33	1.23	3 (11%)
1	CFZ	B	404	1	18,21,22	2.49	7 (38%)	26,30,33	1.24	4 (15%)
1	CFZ	B	242	1	18,21,22	2.50	7 (38%)	26,30,33	1.30	3 (11%)
1	CFZ	B	565	1	18,21,22	2.53	7 (38%)	26,30,33	1.10	3 (11%)
1	CFZ	A	355	1	18,21,22	2.46	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	A	174	1	18,21,22	2.59	9 (50%)	26,30,33	2.00	6 (23%)
1	CFZ	A	387	1	18,21,22	2.52	7 (38%)	26,30,33	1.20	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	B	604	1	18,21,22	2.49	7 (38%)	26,30,33	1.26	3 (11%)
1	UFT	B	175	1	18,21,22	2.60	10 (55%)	26,30,33	1.92	7 (26%)
1	UFT	B	628	1	18,21,22	2.59	10 (55%)	26,30,33	1.98	7 (26%)
1	CFZ	B	498	1	18,21,22	2.47	7 (38%)	26,30,33	1.25	2 (7%)
1	UFT	B	489	1	18,21,22	2.60	9 (50%)	26,30,33	1.81	7 (26%)
1	CFZ	B	664	1	18,21,22	2.47	7 (38%)	26,30,33	1.53	3 (11%)
1	CFZ	B	651	1	18,21,22	2.51	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	A	206	1	18,21,22	2.51	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	B	11	1	18,21,22	2.60	9 (50%)	26,30,33	1.94	8 (30%)
1	CFZ	B	518	1	18,21,22	2.46	7 (38%)	26,30,33	1.37	3 (11%)
1	CFZ	B	161	1	18,21,22	2.48	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	A	229	1	18,21,22	2.62	9 (50%)	26,30,33	1.90	7 (26%)
1	UFT	A	663	1	18,21,22	2.56	9 (50%)	26,30,33	2.09	8 (30%)
1	CFZ	B	246	1	18,21,22	2.53	7 (38%)	26,30,33	1.21	2 (7%)
1	CFZ	B	25	1	18,21,22	2.50	7 (38%)	26,30,33	1.52	3 (11%)
1	UFT	B	182	1	18,21,22	2.57	9 (50%)	26,30,33	2.06	8 (30%)
1	UFT	B	154	1	18,21,22	2.59	10 (55%)	26,30,33	1.99	6 (23%)
1	UFT	B	44	1	18,21,22	2.64	9 (50%)	26,30,33	1.90	7 (26%)
1	UFT	B	431	1	18,21,22	2.58	10 (55%)	26,30,33	2.02	8 (30%)
1	UFT	B	602	1	18,21,22	2.61	9 (50%)	26,30,33	1.87	7 (26%)
1	CFZ	A	373	1	18,21,22	2.49	7 (38%)	26,30,33	1.24	3 (11%)
1	UFT	B	344	1	18,21,22	2.61	9 (50%)	26,30,33	1.88	7 (26%)
1	UFT	B	447	1	18,21,22	2.61	9 (50%)	26,30,33	1.87	7 (26%)
1	CFZ	A	540	1	18,21,22	2.52	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	A	169	1	18,21,22	2.58	10 (55%)	26,30,33	2.00	8 (30%)
1	CFZ	A	117	1	18,21,22	2.46	7 (38%)	26,30,33	1.50	4 (15%)
1	UFT	B	701	1	18,21,22	2.57	9 (50%)	26,30,33	1.97	7 (26%)
1	CFZ	B	110	1	18,21,22	2.51	7 (38%)	26,30,33	1.22	3 (11%)
1	UFT	B	170	1	18,21,22	2.56	10 (55%)	26,30,33	2.11	8 (30%)
1	CFZ	A	201	1	18,21,22	2.49	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	B	554	1	18,21,22	2.59	10 (55%)	26,30,33	2.00	8 (30%)
1	CFZ	A	103	1	18,21,22	2.49	7 (38%)	26,30,33	1.34	3 (11%)
1	UFT	B	106	1	18,21,22	2.58	9 (50%)	26,30,33	1.98	7 (26%)
1	UFT	B	153	1	18,21,22	2.62	9 (50%)	26,30,33	1.88	7 (26%)
1	CFZ	A	603	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	439	1	18,21,22	2.50	7 (38%)	26,30,33	1.53	3 (11%)
1	CFZ	A	469	1	18,21,22	2.47	7 (38%)	26,30,33	1.41	3 (11%)
1	CFZ	B	381	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	A	523	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	637	1	18,21,22	2.47	7 (38%)	26,30,33	1.48	4 (15%)
1	CFZ	B	184	1	18,21,22	2.52	7 (38%)	26,30,33	1.19	2 (7%)
1	UFT	A	609	1	18,21,22	2.57	10 (55%)	26,30,33	2.04	8 (30%)
1	UFT	A	669	1	18,21,22	2.59	9 (50%)	26,30,33	1.88	7 (26%)
1	CFZ	A	353	1	18,21,22	2.47	7 (38%)	26,30,33	1.48	3 (11%)
1	UFT	A	196	1	18,21,22	2.58	9 (50%)	26,30,33	2.01	8 (30%)
1	CFZ	B	285	1	18,21,22	2.53	7 (38%)	26,30,33	1.13	3 (11%)
1	CFZ	A	363	1	18,21,22	2.51	7 (38%)	26,30,33	1.12	3 (11%)
1	UFT	A	155	1	18,21,22	2.58	9 (50%)	26,30,33	1.94	8 (30%)
1	UFT	B	334	1	18,21,22	2.59	9 (50%)	26,30,33	2.01	7 (26%)
1	UFT	A	216	1	18,21,22	2.62	9 (50%)	26,30,33	1.90	7 (26%)
1	UFT	A	84	1	18,21,22	2.59	10 (55%)	26,30,33	1.86	7 (26%)
1	UFT	B	571	1	18,21,22	2.60	9 (50%)	26,30,33	1.94	7 (26%)
1	CFZ	B	439	1	18,21,22	2.48	7 (38%)	26,30,33	1.49	3 (11%)
1	UFT	B	80	1	18,21,22	2.63	9 (50%)	26,30,33	1.86	7 (26%)
1	UFT	B	662	1	18,21,22	2.57	9 (50%)	26,30,33	1.97	8 (30%)
1	UFT	B	456	1	18,21,22	2.62	9 (50%)	26,30,33	1.86	5 (19%)
1	CFZ	A	96	1	18,21,22	2.49	7 (38%)	26,30,33	1.26	2 (7%)
1	CFZ	B	406	1	18,21,22	2.51	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	A	329	1	18,21,22	2.62	9 (50%)	26,30,33	1.87	7 (26%)
1	CFZ	A	325	1	18,21,22	2.52	7 (38%)	26,30,33	1.18	3 (11%)
1	UFT	A	163	1	18,21,22	2.60	9 (50%)	26,30,33	1.89	8 (30%)
1	CFZ	A	369	1	18,21,22	2.50	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	B	621	1	18,21,22	2.56	10 (55%)	26,30,33	2.07	8 (30%)
1	UFT	B	524	1	18,21,22	2.63	9 (50%)	26,30,33	1.87	7 (26%)
1	UFT	B	472	1	18,21,22	2.57	9 (50%)	26,30,33	2.06	6 (23%)
1	UFT	B	245	1	18,21,22	2.63	9 (50%)	26,30,33	1.84	6 (23%)
1	UFT	B	84	1	18,21,22	2.60	9 (50%)	26,30,33	1.94	7 (26%)
1	UFT	B	607	1	18,21,22	2.58	9 (50%)	26,30,33	2.01	7 (26%)
1	UFT	B	305	1	18,21,22	2.56	10 (55%)	26,30,33	1.93	6 (23%)
1	UFT	B	229	1	18,21,22	2.63	9 (50%)	26,30,33	1.85	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	600	1	18,21,22	2.52	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	A	214	1	18,21,22	2.60	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	555	1	18,21,22	2.57	9 (50%)	26,30,33	2.04	6 (23%)
1	CFZ	B	418	1	18,21,22	2.48	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	B	698	1	18,21,22	2.52	7 (38%)	26,30,33	1.19	3 (11%)
1	CFZ	A	679	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	506	1	18,21,22	2.50	7 (38%)	26,30,33	1.34	3 (11%)
1	CFZ	A	486	1	18,21,22	2.48	7 (38%)	26,30,33	1.29	2 (7%)
1	CFZ	A	378	1	18,21,22	2.49	7 (38%)	26,30,33	1.25	3 (11%)
1	UFT	A	690	1	18,21,22	2.60	9 (50%)	26,30,33	1.91	8 (30%)
1	UFT	A	504	1	18,21,22	2.59	10 (55%)	26,30,33	1.94	8 (30%)
1	UFT	B	60	1	18,21,22	2.56	9 (50%)	26,30,33	2.04	8 (30%)
1	CFZ	B	362	1	18,21,22	2.51	7 (38%)	26,30,33	1.43	2 (7%)
1	UFT	A	265	1	18,21,22	2.61	10 (55%)	26,30,33	1.94	7 (26%)
1	UFT	A	204	1	18,21,22	2.60	9 (50%)	26,30,33	1.90	6 (23%)
1	CFZ	A	704	1	18,21,22	2.49	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	A	430	1	18,21,22	2.58	10 (55%)	26,30,33	1.98	8 (30%)
1	UFT	B	535	1	18,21,22	2.64	9 (50%)	26,30,33	1.77	5 (19%)
1	CFZ	B	647	1	18,21,22	2.51	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	A	581	1	18,21,22	2.59	9 (50%)	26,30,33	1.97	7 (26%)
1	UFT	B	636	1	18,21,22	2.58	10 (55%)	26,30,33	2.08	8 (30%)
1	UFT	A	309	1	18,21,22	2.61	9 (50%)	26,30,33	1.93	8 (30%)
1	CFZ	A	518	1	18,21,22	2.51	7 (38%)	26,30,33	1.12	1 (3%)
1	CFZ	A	404	1	18,21,22	2.48	7 (38%)	26,30,33	1.25	4 (15%)
1	CFZ	B	104	1	18,21,22	2.52	7 (38%)	26,30,33	1.16	2 (7%)
1	UFT	A	296	1	18,21,22	2.58	10 (55%)	26,30,33	1.97	8 (30%)
1	UFT	A	179	1	18,21,22	2.63	9 (50%)	26,30,33	1.86	6 (23%)
1	CFZ	B	576	1	18,21,22	2.51	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	A	33	1	18,21,22	2.64	9 (50%)	26,30,33	1.84	7 (26%)
1	CFZ	B	218	1	18,21,22	2.47	7 (38%)	26,30,33	1.28	2 (7%)
1	CFZ	B	156	1	18,21,22	2.51	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	A	551	1	18,21,22	2.52	7 (38%)	26,30,33	1.13	2 (7%)
1	UFT	B	71	1	18,21,22	2.58	9 (50%)	26,30,33	1.94	8 (30%)
1	UFT	A	202	1	18,21,22	2.58	10 (55%)	26,30,33	2.06	7 (26%)
1	UFT	A	86	1	18,21,22	2.60	10 (55%)	26,30,33	1.92	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	B	543	1	18,21,22	2.48	7 (38%)	26,30,33	1.30	3 (11%)
1	UFT	A	8	1	18,21,22	2.61	10 (55%)	26,30,33	1.86	7 (26%)
1	UFT	A	555	1	18,21,22	2.57	10 (55%)	26,30,33	2.06	7 (26%)
1	CFZ	A	383	1	18,21,22	2.50	7 (38%)	26,30,33	1.34	3 (11%)
1	UFT	A	471	1	18,21,22	2.60	9 (50%)	26,30,33	1.85	6 (23%)
1	UFT	A	14	1	18,21,22	2.60	10 (55%)	26,30,33	1.92	6 (23%)
1	UFT	A	481	1	18,21,22	2.59	9 (50%)	26,30,33	1.91	7 (26%)
1	UFT	A	582	1	18,21,22	2.57	10 (55%)	26,30,33	1.97	8 (30%)
1	CFZ	A	592	1	18,21,22	2.49	7 (38%)	26,30,33	1.30	3 (11%)
1	CFZ	A	323	1	18,21,22	2.50	7 (38%)	26,30,33	1.35	2 (7%)
1	CFZ	B	370	1	18,21,22	2.50	7 (38%)	26,30,33	1.26	3 (11%)
1	CFZ	A	28	1	18,21,22	2.49	7 (38%)	26,30,33	1.32	4 (15%)
1	UFT	B	687	1	18,21,22	2.60	9 (50%)	26,30,33	1.91	8 (30%)
1	UFT	A	141	1	18,21,22	2.59	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	A	315	1	18,21,22	2.52	7 (38%)	26,30,33	1.30	2 (7%)
1	CFZ	B	39	1	18,21,22	2.56	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	B	72	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	2 (7%)
1	UFT	B	361	1	18,21,22	2.61	9 (50%)	26,30,33	2.10	7 (26%)
1	UFT	A	673	1	18,21,22	2.60	10 (55%)	26,30,33	2.05	6 (23%)
1	CFZ	A	140	1	18,21,22	2.47	7 (38%)	26,30,33	1.29	2 (7%)
1	CFZ	A	494	1	18,21,22	2.49	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	A	131	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	A	302	1	18,21,22	2.62	9 (50%)	26,30,33	1.94	8 (30%)
1	UFT	B	466	1	18,21,22	2.58	10 (55%)	26,30,33	2.04	8 (30%)
1	UFT	B	437	1	18,21,22	2.56	9 (50%)	26,30,33	1.97	7 (26%)
1	UFT	B	629	1	18,21,22	2.60	9 (50%)	26,30,33	1.85	7 (26%)
1	UFT	A	621	1	18,21,22	2.57	9 (50%)	26,30,33	2.09	8 (30%)
1	CFZ	B	354	1	18,21,22	2.49	7 (38%)	26,30,33	1.35	3 (11%)
1	UFT	B	544	1	18,21,22	2.57	10 (55%)	26,30,33	2.00	6 (23%)
1	UFT	A	313	1	18,21,22	2.63	9 (50%)	26,30,33	1.85	6 (23%)
1	CFZ	A	76	1	18,21,22	2.49	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	A	350	1	18,21,22	2.62	9 (50%)	26,30,33	1.89	7 (26%)
1	CFZ	A	425	1	18,21,22	2.53	7 (38%)	26,30,33	1.21	3 (11%)
1	CFZ	B	120	1	18,21,22	2.53	7 (38%)	26,30,33	1.23	3 (11%)
1	CFZ	A	67	1	18,21,22	2.52	7 (38%)	26,30,33	1.19	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	359	1	18,21,22	2.65	9 (50%)	26,30,33	1.93	8 (30%)
1	CFZ	A	335	1	18,21,22	2.49	7 (38%)	26,30,33	1.36	2 (7%)
1	UFT	A	549	1	18,21,22	2.61	10 (55%)	26,30,33	1.90	6 (23%)
1	CFZ	A	652	1	18,21,22	2.50	7 (38%)	26,30,33	1.23	3 (11%)
1	CFZ	A	657	1	18,21,22	2.43	7 (38%)	26,30,33	1.27	3 (11%)
1	CFZ	A	451	1	18,21,22	2.49	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	B	130	1	18,21,22	2.50	7 (38%)	26,30,33	1.23	2 (7%)
1	CFZ	A	151	1	18,21,22	2.51	7 (38%)	26,30,33	1.25	3 (11%)
1	UFT	A	97	1	18,21,22	2.59	9 (50%)	26,30,33	1.90	7 (26%)
1	CFZ	A	57	1	18,21,22	2.50	7 (38%)	26,30,33	1.14	3 (11%)
1	CFZ	B	438	1	18,21,22	2.48	7 (38%)	26,30,33	1.45	4 (15%)
1	CFZ	B	492	1	18,21,22	2.52	8 (44%)	26,30,33	1.14	2 (7%)
1	UFT	B	581	1	18,21,22	2.59	9 (50%)	26,30,33	1.97	7 (26%)
1	CFZ	A	579	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	UFT	A	719	1	18,21,22	2.58	10 (55%)	26,30,33	2.10	6 (23%)
1	CFZ	A	693	1	18,21,22	2.51	7 (38%)	26,30,33	1.19	2 (7%)
1	CFZ	A	583	1	18,21,22	2.47	7 (38%)	26,30,33	1.48	4 (15%)
1	CFZ	A	338	1	18,21,22	2.50	7 (38%)	26,30,33	1.41	2 (7%)
1	CFZ	A	585	1	18,21,22	2.51	7 (38%)	26,30,33	1.24	3 (11%)
1	UFT	B	669	1	18,21,22	2.61	9 (50%)	26,30,33	1.87	7 (26%)
1	UFT	A	112	1	18,21,22	2.59	10 (55%)	26,30,33	1.89	8 (30%)
1	CFZ	B	117	1	18,21,22	2.46	7 (38%)	26,30,33	1.50	4 (15%)
1	UFT	B	179	1	18,21,22	2.64	9 (50%)	26,30,33	1.88	6 (23%)
1	CFZ	A	370	1	18,21,22	2.51	7 (38%)	26,30,33	1.26	3 (11%)
1	CFZ	A	285	1	18,21,22	2.52	7 (38%)	26,30,33	1.13	3 (11%)
1	UFT	B	689	1	18,21,22	2.59	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	B	338	1	18,21,22	2.47	7 (38%)	26,30,33	1.46	2 (7%)
1	CFZ	B	279	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	B	666	1	18,21,22	2.58	10 (55%)	26,30,33	1.95	8 (30%)
1	CFZ	A	171	1	18,21,22	2.47	7 (38%)	26,30,33	1.50	4 (15%)
1	UFT	B	174	1	18,21,22	2.59	9 (50%)	26,30,33	2.02	6 (23%)
1	CFZ	A	282	1	18,21,22	2.49	7 (38%)	26,30,33	1.40	3 (11%)
1	UFT	A	260	1	18,21,22	2.63	9 (50%)	26,30,33	1.85	6 (23%)
1	CFZ	A	528	1	18,21,22	2.54	7 (38%)	26,30,33	1.20	3 (11%)
1	CFZ	A	637	1	18,21,22	2.47	7 (38%)	26,30,33	1.49	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	B	169	1	18,21,22	2.57	9 (50%)	26,30,33	2.01	8 (30%)
1	CFZ	A	625	1	18,21,22	2.50	7 (38%)	26,30,33	1.33	3 (11%)
1	UFT	A	608	1	18,21,22	2.57	9 (50%)	26,30,33	1.98	8 (30%)
1	CFZ	A	655	1	18,21,22	2.51	7 (38%)	26,30,33	1.47	3 (11%)
1	CFZ	B	600	1	18,21,22	2.52	7 (38%)	26,30,33	1.19	3 (11%)
1	CFZ	B	140	1	18,21,22	2.46	7 (38%)	26,30,33	1.29	2 (7%)
1	CFZ	B	131	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	B	377	1	18,21,22	2.61	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	A	517	1	18,21,22	2.48	7 (38%)	26,30,33	1.55	3 (11%)
1	CFZ	A	63	1	18,21,22	2.46	7 (38%)	26,30,33	1.49	4 (15%)
1	UFT	B	197	1	18,21,22	2.57	10 (55%)	26,30,33	2.00	8 (30%)
1	UFT	B	135	1	18,21,22	2.62	9 (50%)	26,30,33	1.90	6 (23%)
1	UFT	A	500	1	18,21,22	2.57	10 (55%)	26,30,33	2.02	8 (30%)
1	UFT	B	74	1	18,21,22	2.56	9 (50%)	26,30,33	2.06	8 (30%)
1	CFZ	B	426	1	18,21,22	2.51	7 (38%)	26,30,33	1.26	3 (11%)
1	CFZ	A	418	1	18,21,22	2.47	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	B	316	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	2 (7%)
1	CFZ	A	492	1	18,21,22	2.49	7 (38%)	26,30,33	1.39	3 (11%)
1	UFT	A	653	1	18,21,22	2.60	9 (50%)	26,30,33	1.93	8 (30%)
1	UFT	B	389	1	18,21,22	2.62	9 (50%)	26,30,33	1.87	6 (23%)
1	CFZ	A	156	1	18,21,22	2.52	7 (38%)	26,30,33	1.27	3 (11%)
1	CFZ	A	498	1	18,21,22	2.48	7 (38%)	26,30,33	1.25	2 (7%)
1	CFZ	B	399	1	18,21,22	2.50	7 (38%)	26,30,33	1.30	3 (11%)
1	CFZ	A	667	1	18,21,22	2.49	7 (38%)	26,30,33	1.30	3 (11%)
1	UFT	B	423	1	18,21,22	2.62	10 (55%)	26,30,33	1.92	7 (26%)
1	UFT	B	606	1	18,21,22	2.55	10 (55%)	26,30,33	2.08	8 (30%)
1	UFT	B	633	1	18,21,22	2.60	10 (55%)	26,30,33	1.89	7 (26%)
1	CFZ	A	473	1	18,21,22	2.48	7 (38%)	26,30,33	1.25	3 (11%)
1	UFT	A	703	1	18,21,22	2.62	9 (50%)	26,30,33	1.84	5 (19%)
1	UFT	B	398	1	18,21,22	2.60	10 (55%)	26,30,33	1.94	8 (30%)
1	CFZ	A	459	1	18,21,22	2.47	7 (38%)	26,30,33	1.33	3 (11%)
1	CFZ	B	585	1	18,21,22	2.51	7 (38%)	26,30,33	1.22	3 (11%)
1	UFT	A	554	1	18,21,22	2.59	10 (55%)	26,30,33	1.95	8 (30%)
1	UFT	A	434	1	18,21,22	2.57	9 (50%)	26,30,33	1.99	8 (30%)
1	CFZ	A	49	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	B	325	1	18,21,22	2.50	7 (38%)	26,30,33	1.27	3 (11%)
1	CFZ	B	511	1	18,21,22	2.52	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	A	105	1	18,21,22	2.58	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	A	351	1	18,21,22	2.48	7 (38%)	26,30,33	1.19	3 (11%)
1	UFT	B	108	1	18,21,22	2.65	9 (50%)	26,30,33	1.81	5 (19%)
1	UFT	B	421	1	18,21,22	2.62	9 (50%)	26,30,33	1.89	7 (26%)
1	UFT	A	687	1	18,21,22	2.60	9 (50%)	26,30,33	1.90	8 (30%)
1	CFZ	A	444	1	18,21,22	2.47	7 (38%)	26,30,33	1.44	4 (15%)
1	UFT	A	629	1	18,21,22	2.61	9 (50%)	26,30,33	1.85	7 (26%)
1	UFT	A	447	1	18,21,22	2.61	9 (50%)	26,30,33	1.87	7 (26%)
1	UFT	B	214	1	18,21,22	2.60	9 (50%)	26,30,33	1.91	8 (30%)
1	UFT	B	464	1	18,21,22	2.63	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	352	1	18,21,22	2.63	9 (50%)	26,30,33	1.92	7 (26%)
1	CFZ	B	407	1	18,21,22	2.49	7 (38%)	26,30,33	1.23	3 (11%)
1	CFZ	B	315	1	18,21,22	2.50	7 (38%)	26,30,33	1.32	2 (7%)
1	UFT	A	402	1	18,21,22	2.60	10 (55%)	26,30,33	1.90	7 (26%)
1	CFZ	A	130	1	18,21,22	2.51	7 (38%)	26,30,33	1.23	2 (7%)
1	CFZ	B	491	1	18,21,22	2.55	7 (38%)	26,30,33	1.16	4 (15%)
1	UFT	B	266	1	18,21,22	2.59	10 (55%)	26,30,33	1.96	8 (30%)
1	CFZ	A	15	1	18,21,22	2.45	7 (38%)	26,30,33	1.38	3 (11%)
1	UFT	B	673	1	18,21,22	2.59	9 (50%)	26,30,33	2.06	6 (23%)
1	CFZ	A	446	1	18,21,22	2.50	7 (38%)	26,30,33	1.43	3 (11%)
1	CFZ	B	424	1	18,21,22	2.51	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	A	503	1	18,21,22	2.58	10 (55%)	26,30,33	2.00	7 (26%)
1	CFZ	B	592	1	18,21,22	2.47	7 (38%)	26,30,33	1.27	2 (7%)
1	CFZ	B	512	1	18,21,22	2.52	7 (38%)	26,30,33	1.12	1 (3%)
1	CFZ	B	209	1	18,21,22	2.52	7 (38%)	26,30,33	1.16	2 (7%)
1	UFT	A	208	1	18,21,22	2.62	9 (50%)	26,30,33	1.89	8 (30%)
1	CFZ	A	440	1	18,21,22	2.47	7 (38%)	26,30,33	1.44	3 (11%)
1	UFT	B	43	1	18,21,22	2.62	9 (50%)	26,30,33	2.12	9 (34%)
1	UFT	B	32	1	18,21,22	2.61	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	703	1	18,21,22	2.62	9 (50%)	26,30,33	1.81	5 (19%)
1	UFT	B	33	1	18,21,22	2.62	9 (50%)	26,30,33	1.87	6 (23%)
1	CFZ	A	232	1	18,21,22	2.49	7 (38%)	26,30,33	1.28	4 (15%)
1	CFZ	A	234	1	18,21,22	2.48	7 (38%)	26,30,33	1.37	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	32	1	18,21,22	2.60	11 (61%)	26,30,33	1.93	8 (30%)
1	CFZ	B	459	1	18,21,22	2.48	7 (38%)	26,30,33	1.33	3 (11%)
1	UFT	A	676	1	18,21,22	2.64	9 (50%)	26,30,33	1.94	7 (26%)
1	UFT	A	712	1	18,21,22	2.62	9 (50%)	26,30,33	1.87	7 (26%)
1	UFT	A	108	1	18,21,22	2.65	9 (50%)	26,30,33	1.81	5 (19%)
1	UFT	A	646	1	18,21,22	2.60	9 (50%)	26,30,33	1.99	6 (23%)
1	UFT	B	430	1	18,21,22	2.58	9 (50%)	26,30,33	1.98	7 (26%)
1	CFZ	B	129	1	18,21,22	2.53	7 (38%)	26,30,33	1.10	1 (3%)
1	CFZ	B	247	1	18,21,22	2.52	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	A	344	1	18,21,22	2.60	10 (55%)	26,30,33	1.98	7 (26%)
1	UFT	A	19	1	18,21,22	2.60	10 (55%)	26,30,33	1.95	8 (30%)
1	UFT	A	50	1	18,21,22	2.63	9 (50%)	26,30,33	1.86	6 (23%)
1	CFZ	B	378	1	18,21,22	2.50	7 (38%)	26,30,33	1.25	3 (11%)
1	UFT	B	471	1	18,21,22	2.60	9 (50%)	26,30,33	1.84	6 (23%)
1	UFT	B	481	1	18,21,22	2.58	9 (50%)	26,30,33	1.92	7 (26%)
1	CFZ	A	384	1	18,21,22	2.50	7 (38%)	26,30,33	1.32	3 (11%)
1	UFT	A	684	1	18,21,22	2.63	9 (50%)	26,30,33	1.82	6 (23%)
1	UFT	A	659	1	18,21,22	2.63	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	A	241	1	18,21,22	2.47	7 (38%)	26,30,33	1.57	4 (15%)
1	CFZ	B	321	1	18,21,22	2.45	7 (38%)	26,30,33	1.43	3 (11%)
1	CFZ	A	568	1	18,21,22	2.53	7 (38%)	26,30,33	1.21	3 (11%)
1	CFZ	B	631	1	18,21,22	2.51	7 (38%)	26,30,33	1.35	3 (11%)
1	UFT	B	542	1	18,21,22	2.59	10 (55%)	26,30,33	1.93	7 (26%)
1	CFZ	A	321	1	18,21,22	2.49	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	A	587	1	18,21,22	2.51	7 (38%)	26,30,33	1.18	3 (11%)
1	UFT	A	217	1	18,21,22	2.62	9 (50%)	26,30,33	1.89	7 (26%)
1	CFZ	B	568	1	18,21,22	2.52	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	A	398	1	18,21,22	2.59	10 (55%)	26,30,33	1.94	8 (30%)
1	CFZ	B	234	1	18,21,22	2.48	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	B	190	1	18,21,22	2.58	9 (50%)	26,30,33	2.00	8 (30%)
1	CFZ	B	536	1	18,21,22	2.47	7 (38%)	26,30,33	1.50	3 (11%)
1	CFZ	A	647	1	18,21,22	2.52	7 (38%)	26,30,33	1.21	3 (11%)
1	CFZ	B	639	1	18,21,22	2.49	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	B	587	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	A	73	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	B	359	1	18,21,22	2.60	10 (55%)	26,30,33	1.93	8 (30%)
1	UFT	B	283	1	18,21,22	2.62	9 (50%)	26,30,33	1.88	6 (23%)
1	UFT	B	366	1	18,21,22	2.57	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	A	426	1	18,21,22	2.51	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	B	534	1	18,21,22	2.61	10 (55%)	26,30,33	1.88	7 (26%)
1	CFZ	B	657	1	18,21,22	2.42	7 (38%)	26,30,33	1.26	3 (11%)
1	UFT	B	55	1	18,21,22	2.60	9 (50%)	26,30,33	1.90	7 (26%)
1	UFT	A	192	1	18,21,22	2.62	10 (55%)	26,30,33	1.87	7 (26%)
1	CFZ	A	120	1	18,21,22	2.52	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	124	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	3 (11%)
1	CFZ	A	682	1	18,21,22	2.51	7 (38%)	26,30,33	1.21	2 (7%)
1	CFZ	B	383	1	18,21,22	2.48	7 (38%)	26,30,33	1.17	2 (7%)
1	UFT	A	618	1	18,21,22	2.57	9 (50%)	26,30,33	2.03	8 (30%)
1	UFT	A	666	1	18,21,22	2.58	9 (50%)	26,30,33	1.96	8 (30%)
1	CFZ	B	579	1	18,21,22	2.51	7 (38%)	26,30,33	1.22	3 (11%)
1	UFT	A	293	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	6 (23%)
1	CFZ	B	441	1	18,21,22	2.53	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	A	328	1	18,21,22	2.48	7 (38%)	26,30,33	1.46	2 (7%)
1	UFT	A	628	1	18,21,22	2.58	10 (55%)	26,30,33	1.98	7 (26%)
1	UFT	A	137	1	18,21,22	2.60	10 (55%)	26,30,33	1.91	8 (30%)
1	UFT	B	98	1	18,21,22	2.61	10 (55%)	26,30,33	1.94	8 (30%)
1	UFT	B	301	1	18,21,22	2.57	10 (55%)	26,30,33	1.99	8 (30%)
1	UFT	A	485	1	18,21,22	2.60	10 (55%)	26,30,33	1.94	6 (23%)
1	CFZ	B	548	1	18,21,22	2.50	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	A	399	1	18,21,22	2.50	7 (38%)	26,30,33	1.31	3 (11%)
1	CFZ	B	332	1	18,21,22	2.49	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	B	530	1	18,21,22	2.59	9 (50%)	26,30,33	1.97	7 (26%)
1	UFT	B	656	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	7 (26%)
1	UFT	B	48	1	18,21,22	2.59	10 (55%)	26,30,33	2.01	6 (23%)
1	UFT	A	44	1	18,21,22	2.63	9 (50%)	26,30,33	1.87	7 (26%)
1	CFZ	B	282	1	18,21,22	2.50	7 (38%)	26,30,33	1.38	3 (11%)
1	UFT	B	296	1	18,21,22	2.58	10 (55%)	26,30,33	1.97	8 (30%)
1	UFT	A	89	1	18,21,22	2.57	9 (50%)	26,30,33	2.04	8 (30%)
1	UFT	A	544	1	18,21,22	2.57	9 (50%)	26,30,33	2.00	6 (23%)
1	UFT	A	11	1	18,21,22	2.60	10 (55%)	26,30,33	1.86	8 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	B	593	1	18,21,22	2.54	9 (50%)	26,30,33	1.93	8 (30%)
1	UFT	A	352	1	18,21,22	2.57	9 (50%)	26,30,33	2.00	8 (30%)
1	UFT	B	712	1	18,21,22	2.61	10 (55%)	26,30,33	1.84	6 (23%)
1	CFZ	A	46	1	18,21,22	2.52	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	A	432	1	18,21,22	2.61	10 (55%)	26,30,33	1.85	5 (19%)
1	CFZ	A	565	1	18,21,22	2.53	7 (38%)	26,30,33	1.10	3 (11%)
1	CFZ	B	655	1	18,21,22	2.51	7 (38%)	26,30,33	1.46	3 (11%)
1	UFT	A	365	1	18,21,22	2.63	9 (50%)	26,30,33	1.87	6 (23%)
1	CFZ	A	304	1	18,21,22	2.52	7 (38%)	26,30,33	1.14	3 (11%)
1	UFT	A	431	1	18,21,22	2.59	10 (55%)	26,30,33	2.02	8 (30%)
1	CFZ	A	124	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	3 (11%)
1	CFZ	B	79	1	18,21,22	2.49	7 (38%)	26,30,33	1.35	3 (11%)
1	UFT	B	200	1	18,21,22	2.56	10 (55%)	26,30,33	2.01	7 (26%)
1	CFZ	B	198	1	18,21,22	2.49	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	A	43	1	18,21,22	2.62	9 (50%)	26,30,33	2.10	9 (34%)
1	CFZ	A	474	1	18,21,22	2.51	7 (38%)	26,30,33	1.25	3 (11%)
1	CFZ	B	75	1	18,21,22	2.49	7 (38%)	26,30,33	1.39	2 (7%)
1	UFT	B	347	1	18,21,22	2.58	9 (50%)	26,30,33	1.99	6 (23%)
1	UFT	A	182	1	18,21,22	2.56	9 (50%)	26,30,33	2.05	7 (26%)
1	UFT	B	653	1	18,21,22	2.57	9 (50%)	26,30,33	1.95	8 (30%)
1	UFT	B	367	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	6 (23%)
1	UFT	B	590	1	18,21,22	2.60	9 (50%)	26,30,33	2.00	6 (23%)
1	UFT	B	251	1	18,21,22	2.62	10 (55%)	26,30,33	1.88	8 (30%)
1	UFT	A	175	1	18,21,22	2.60	9 (50%)	26,30,33	1.91	7 (26%)
1	UFT	B	322	1	18,21,22	2.61	9 (50%)	26,30,33	1.88	7 (26%)
1	CFZ	B	26	1	18,21,22	2.45	7 (38%)	26,30,33	1.33	3 (11%)
1	UFT	A	334	1	18,21,22	2.58	9 (50%)	26,30,33	2.01	7 (26%)
1	CFZ	A	691	1	18,21,22	2.48	7 (38%)	26,30,33	1.30	3 (11%)
1	UFT	B	493	1	18,21,22	2.66	9 (50%)	26,30,33	1.83	7 (26%)
1	CFZ	A	210	1	18,21,22	2.48	7 (38%)	26,30,33	1.37	3 (11%)
1	CFZ	A	184	1	18,21,22	2.52	7 (38%)	26,30,33	1.18	2 (7%)
1	UFT	A	456	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	5 (19%)
1	CFZ	B	49	1	18,21,22	2.53	7 (38%)	26,30,33	1.16	4 (15%)
1	CFZ	A	436	1	18,21,22	2.52	7 (38%)	26,30,33	1.22	2 (7%)
1	UFT	B	577	1	18,21,22	2.61	10 (55%)	26,30,33	1.87	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	411	1	18,21,22	2.50	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	B	708	1	18,21,22	2.61	9 (50%)	26,30,33	1.88	7 (26%)
1	UFT	B	196	1	18,21,22	2.59	9 (50%)	26,30,33	2.01	8 (30%)
1	UFT	A	696	1	18,21,22	2.58	9 (50%)	26,30,33	1.96	8 (30%)
1	UFT	A	472	1	18,21,22	2.58	9 (50%)	26,30,33	2.02	6 (23%)
1	CFZ	A	279	1	18,21,22	2.53	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	A	116	1	18,21,22	2.58	9 (50%)	26,30,33	2.07	8 (30%)
1	UFT	B	115	1	18,21,22	2.58	9 (50%)	26,30,33	2.00	8 (30%)
1	CFZ	A	242	1	18,21,22	2.51	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	B	336	1	18,21,22	2.59	10 (55%)	26,30,33	1.98	8 (30%)
1	CFZ	A	556	1	18,21,22	2.48	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	B	86	1	18,21,22	2.60	10 (55%)	26,30,33	1.90	8 (30%)
1	UFT	A	336	1	18,21,22	2.58	9 (50%)	26,30,33	1.97	8 (30%)
1	CFZ	A	382	1	18,21,22	2.47	7 (38%)	26,30,33	1.38	2 (7%)
1	CFZ	B	171	1	18,21,22	2.46	7 (38%)	26,30,33	1.50	4 (15%)
1	UFT	B	502	1	18,21,22	2.60	10 (55%)	26,30,33	2.00	6 (23%)
1	UFT	B	545	1	18,21,22	2.61	9 (50%)	26,30,33	1.91	7 (26%)
1	UFT	B	163	1	18,21,22	2.61	9 (50%)	26,30,33	1.90	8 (30%)
1	CFZ	A	698	1	18,21,22	2.52	7 (38%)	26,30,33	1.18	3 (11%)
1	UFT	A	59	1	18,21,22	2.60	10 (55%)	26,30,33	1.92	7 (26%)
1	UFT	A	170	1	18,21,22	2.57	9 (50%)	26,30,33	2.11	8 (30%)
1	UFT	A	283	1	18,21,22	2.62	9 (50%)	26,30,33	1.89	6 (23%)
1	UFT	B	89	1	18,21,22	2.57	10 (55%)	26,30,33	2.04	8 (30%)
1	UFT	B	432	1	18,21,22	2.61	9 (50%)	26,30,33	1.87	5 (19%)
1	UFT	A	270	1	18,21,22	2.57	10 (55%)	26,30,33	2.03	7 (26%)
1	UFT	A	197	1	18,21,22	2.58	9 (50%)	26,30,33	2.00	8 (30%)
1	CFZ	B	63	1	18,21,22	2.47	7 (38%)	26,30,33	1.49	4 (15%)
1	CFZ	B	15	1	18,21,22	2.44	7 (38%)	26,30,33	1.39	3 (11%)
1	UFT	B	62	1	18,21,22	2.58	9 (50%)	26,30,33	2.05	8 (30%)
1	CFZ	B	212	1	18,21,22	2.49	7 (38%)	26,30,33	1.33	3 (11%)
1	CFZ	B	360	1	18,21,22	2.46	7 (38%)	26,30,33	1.40	3 (11%)
1	UFT	A	606	1	18,21,22	2.57	10 (55%)	26,30,33	2.07	7 (26%)
1	CFZ	A	188	1	18,21,22	2.52	7 (38%)	26,30,33	1.18	3 (11%)
1	CFZ	B	363	1	18,21,22	2.52	7 (38%)	26,30,33	1.11	2 (7%)
1	CFZ	A	212	1	18,21,22	2.48	7 (38%)	26,30,33	1.32	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	B	425	1	18,21,22	2.52	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	351	1	18,21,22	2.51	7 (38%)	26,30,33	1.19	3 (11%)
1	UFT	B	97	1	18,21,22	2.60	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	265	1	18,21,22	2.61	9 (50%)	26,30,33	1.95	7 (26%)
1	UFT	A	656	1	18,21,22	2.57	9 (50%)	26,30,33	1.96	7 (26%)
1	CFZ	A	218	1	18,21,22	2.47	7 (38%)	26,30,33	1.28	2 (7%)
1	UFT	B	646	1	18,21,22	2.61	9 (50%)	26,30,33	1.98	6 (23%)
1	CFZ	B	34	1	18,21,22	2.48	7 (38%)	26,30,33	1.32	3 (11%)
1	CFZ	A	381	1	18,21,22	2.51	7 (38%)	26,30,33	1.31	2 (7%)
1	UFT	B	434	1	18,21,22	2.58	10 (55%)	26,30,33	2.01	8 (30%)
1	UFT	A	602	1	18,21,22	2.61	10 (55%)	26,30,33	1.88	7 (26%)
1	CFZ	B	693	1	18,21,22	2.51	7 (38%)	26,30,33	1.18	2 (7%)
1	CFZ	B	355	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	4 (15%)
1	CFZ	B	405	1	18,21,22	2.50	7 (38%)	26,30,33	1.30	3 (11%)
1	UFT	A	60	1	18,21,22	2.55	9 (50%)	26,30,33	1.98	7 (26%)
1	UFT	A	464	1	18,21,22	2.63	9 (50%)	26,30,33	1.91	7 (26%)
1	CFZ	B	384	1	18,21,22	2.47	7 (38%)	26,30,33	1.41	2 (7%)
1	UFT	A	13	1	18,21,22	2.55	9 (50%)	26,30,33	2.04	7 (26%)
1	CFZ	A	268	1	18,21,22	2.48	7 (38%)	26,30,33	1.49	2 (7%)
1	UFT	B	329	1	18,21,22	2.60	10 (55%)	26,30,33	1.88	8 (30%)
1	CFZ	B	373	1	18,21,22	2.49	7 (38%)	26,30,33	1.24	3 (11%)
1	CFZ	A	72	1	18,21,22	2.50	7 (38%)	26,30,33	1.26	3 (11%)
1	CFZ	B	206	1	18,21,22	2.51	7 (38%)	26,30,33	1.26	3 (11%)
1	CFZ	A	506	1	18,21,22	2.50	7 (38%)	26,30,33	1.33	3 (11%)
1	UFT	B	582	1	18,21,22	2.58	9 (50%)	26,30,33	1.98	8 (30%)
1	UFT	B	233	1	18,21,22	2.63	10 (55%)	26,30,33	1.81	6 (23%)
1	CFZ	B	232	1	18,21,22	2.46	7 (38%)	26,30,33	1.37	4 (15%)
1	CFZ	A	149	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	A	61	1	18,21,22	2.58	9 (50%)	26,30,33	2.02	8 (30%)
1	CFZ	B	165	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	2 (7%)
1	UFT	A	389	1	18,21,22	2.64	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	A	354	1	18,21,22	2.46	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	A	266	1	18,21,22	2.61	10 (55%)	26,30,33	1.96	7 (26%)
1	UFT	A	499	1	18,21,22	2.61	9 (50%)	26,30,33	1.90	7 (26%)
1	CFZ	B	103	1	18,21,22	2.50	7 (38%)	26,30,33	1.32	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	104	1	18,21,22	2.53	7 (38%)	26,30,33	1.18	3 (11%)
1	CFZ	B	682	1	18,21,22	2.53	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	A	571	1	18,21,22	2.61	10 (55%)	26,30,33	1.94	7 (26%)
1	UFT	B	88	1	18,21,22	2.59	10 (55%)	26,30,33	1.94	8 (30%)
1	UFT	B	609	1	18,21,22	2.57	10 (55%)	26,30,33	2.07	8 (30%)
1	CFZ	A	651	1	18,21,22	2.49	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	A	361	1	18,21,22	2.59	9 (50%)	26,30,33	1.93	7 (26%)
1	CFZ	B	465	1	18,21,22	2.48	7 (38%)	26,30,33	1.30	2 (7%)
1	UFT	B	69	1	18,21,22	2.57	9 (50%)	26,30,33	2.01	7 (26%)
1	UFT	B	676	1	18,21,22	2.63	9 (50%)	26,30,33	1.93	7 (26%)
1	UFT	A	154	1	18,21,22	2.59	9 (50%)	26,30,33	1.99	6 (23%)
1	CFZ	A	26	1	18,21,22	2.48	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	A	491	1	18,21,22	2.50	7 (38%)	26,30,33	1.29	3 (11%)
1	CFZ	A	610	1	18,21,22	2.47	7 (38%)	26,30,33	1.45	4 (15%)
1	CFZ	B	323	1	18,21,22	2.51	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	201	1	18,21,22	2.49	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	B	513	1	18,21,22	2.66	9 (50%)	26,30,33	1.79	6 (23%)
1	UFT	A	577	1	18,21,22	2.60	10 (55%)	26,30,33	1.88	7 (26%)
1	UFT	B	659	1	18,21,22	2.63	9 (50%)	26,30,33	1.86	7 (26%)
1	UFT	A	305	1	18,21,22	2.55	9 (50%)	26,30,33	1.95	6 (23%)
1	UFT	A	466	1	18,21,22	2.58	10 (55%)	26,30,33	2.04	7 (26%)
1	CFZ	B	111	1	18,21,22	2.49	7 (38%)	26,30,33	1.37	3 (11%)
1	CFZ	B	96	1	18,21,22	2.47	7 (38%)	26,30,33	1.40	3 (11%)
1	CFZ	A	39	1	18,21,22	2.56	7 (38%)	26,30,33	1.18	3 (11%)
1	CFZ	B	369	1	18,21,22	2.50	7 (38%)	26,30,33	1.31	3 (11%)
1	CFZ	A	512	1	18,21,22	2.50	7 (38%)	26,30,33	1.13	2 (7%)
1	CFZ	B	704	1	18,21,22	2.50	7 (38%)	26,30,33	1.27	3 (11%)
1	UFT	B	559	1	18,21,22	2.60	9 (50%)	26,30,33	1.96	7 (26%)
1	UFT	B	519	1	18,21,22	2.60	9 (50%)	26,30,33	1.99	8 (30%)
1	UFT	A	92	1	18,21,22	2.61	9 (50%)	26,30,33	1.85	7 (26%)
1	UFT	A	106	1	18,21,22	2.59	9 (50%)	26,30,33	1.99	7 (26%)
1	CFZ	B	304	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	3 (11%)
1	CFZ	A	360	1	18,21,22	2.50	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	A	437	1	18,21,22	2.55	9 (50%)	26,30,33	1.97	7 (26%)
1	CFZ	B	469	1	18,21,22	2.47	7 (38%)	26,30,33	1.42	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	B	523	1	18,21,22	2.49	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	B	260	1	18,21,22	2.63	9 (50%)	26,30,33	1.85	6 (23%)
1	CFZ	A	558	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	3 (11%)
1	CFZ	B	474	1	18,21,22	2.49	7 (38%)	26,30,33	1.25	3 (11%)
1	UFT	B	208	1	18,21,22	2.62	9 (50%)	26,30,33	1.88	6 (23%)
1	CFZ	B	46	1	18,21,22	2.53	7 (38%)	26,30,33	1.14	3 (11%)
1	UFT	B	608	1	18,21,22	2.56	10 (55%)	26,30,33	2.09	8 (30%)
1	CFZ	A	700	1	18,21,22	2.50	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	B	192	1	18,21,22	2.62	10 (55%)	26,30,33	1.85	7 (26%)
1	UFT	A	69	1	18,21,22	2.57	10 (55%)	26,30,33	2.03	8 (30%)
1	CFZ	A	424	1	18,21,22	2.53	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	A	423	1	18,21,22	2.60	9 (50%)	26,30,33	1.92	7 (26%)
1	UFT	B	460	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	B	517	1	18,21,22	2.51	7 (38%)	26,30,33	1.35	2 (7%)
1	CFZ	A	249	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	A	406	1	18,21,22	2.52	7 (38%)	26,30,33	1.28	3 (11%)
1	CFZ	B	149	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	528	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	A	550	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	2 (7%)
1	CFZ	B	353	1	18,21,22	2.47	7 (38%)	26,30,33	1.45	4 (15%)
1	CFZ	B	691	1	18,21,22	2.47	7 (38%)	26,30,33	1.30	3 (11%)
1	UFT	A	502	1	18,21,22	2.59	9 (50%)	26,30,33	1.99	6 (23%)
1	CFZ	B	550	1	18,21,22	2.52	7 (38%)	26,30,33	1.18	2 (7%)
1	UFT	B	216	1	18,21,22	2.65	9 (50%)	26,30,33	1.89	7 (26%)
1	CFZ	A	161	1	18,21,22	2.49	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	A	607	1	18,21,22	2.60	9 (50%)	26,30,33	1.90	8 (30%)
1	UFT	B	403	1	18,21,22	2.58	10 (55%)	26,30,33	1.98	8 (30%)
1	UFT	A	80	1	18,21,22	2.62	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	A	362	1	18,21,22	2.46	7 (38%)	26,30,33	1.39	3 (11%)
1	CFZ	B	254	1	18,21,22	2.48	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	B	112	1	18,21,22	2.59	10 (55%)	26,30,33	1.91	8 (30%)
1	CFZ	A	34	1	18,21,22	2.51	7 (38%)	26,30,33	1.30	3 (11%)
1	CFZ	B	551	1	18,21,22	2.53	7 (38%)	26,30,33	1.12	2 (7%)
1	UFT	B	696	1	18,21,22	2.58	9 (50%)	26,30,33	1.96	8 (30%)
1	CFZ	B	473	1	18,21,22	2.46	7 (38%)	26,30,33	1.34	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	B	144	1	18,21,22	2.47	7 (38%)	26,30,33	1.52	3 (11%)
1	UFT	A	509	1	18,21,22	2.62	10 (55%)	26,30,33	1.93	7 (26%)
1	CFZ	A	477	1	18,21,22	2.51	7 (38%)	26,30,33	1.15	3 (11%)
1	UFT	A	534	1	18,21,22	2.62	10 (55%)	26,30,33	1.88	7 (26%)
1	UFT	A	535	1	18,21,22	2.65	9 (50%)	26,30,33	1.75	5 (19%)
1	UFT	B	8	1	18,21,22	2.63	9 (50%)	26,30,33	2.04	6 (23%)
1	UFT	B	101	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	8 (30%)
1	CFZ	B	28	1	18,21,22	2.49	7 (38%)	26,30,33	1.95	4 (15%)
1	CFZ	A	574	1	18,21,22	2.49	7 (38%)	26,30,33	1.14	3 (11%)
1	UFT	B	160	1	18,21,22	2.57	10 (55%)	26,30,33	1.99	8 (30%)
1	CFZ	B	387	1	18,21,22	2.52	7 (38%)	26,30,33	1.11	1 (3%)
1	UFT	B	720	1	18,21,22	2.62	9 (50%)	26,30,33	1.79	4 (15%)
1	CFZ	A	209	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	2 (7%)
1	UFT	A	708	1	18,21,22	2.59	9 (50%)	26,30,33	1.88	7 (26%)
1	CFZ	A	441	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	B	188	1	18,21,22	2.51	7 (38%)	26,30,33	1.18	3 (11%)
1	CFZ	B	494	1	18,21,22	2.54	6 (33%)	26,30,33	1.27	2 (7%)
1	UFT	A	48	1	18,21,22	2.58	9 (50%)	26,30,33	2.02	6 (23%)
1	CFZ	A	219	1	18,21,22	2.52	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	B	114	1	18,21,22	2.48	7 (38%)	26,30,33	1.45	4 (15%)
1	CFZ	B	73	1	18,21,22	2.51	7 (38%)	26,30,33	1.21	2 (7%)
1	UFT	A	590	1	18,21,22	2.56	9 (50%)	26,30,33	2.02	6 (23%)
1	CFZ	A	164	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	CFZ	B	574	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	3 (11%)
1	CFZ	B	632	1	18,21,22	2.49	7 (38%)	26,30,33	1.25	2 (7%)
1	CFZ	A	139	1	18,21,22	2.50	7 (38%)	26,30,33	1.31	3 (11%)
1	UFT	A	519	1	18,21,22	2.51	9 (50%)	26,30,33	2.01	8 (30%)
1	CFZ	A	511	1	18,21,22	2.52	7 (38%)	26,30,33	1.20	2 (7%)
1	UFT	A	94	1	18,21,22	2.59	9 (50%)	26,30,33	2.00	7 (26%)
1	CFZ	A	620	1	18,21,22	2.49	7 (38%)	26,30,33	1.37	3 (11%)
1	UFT	A	720	1	18,21,22	2.59	9 (50%)	26,30,33	1.97	8 (30%)
1	CFZ	B	10	1	18,21,22	2.46	7 (38%)	26,30,33	1.28	2 (7%)
1	CFZ	A	129	1	18,21,22	2.53	7 (38%)	26,30,33	1.10	1 (3%)
1	UFT	A	421	1	18,21,22	2.61	10 (55%)	26,30,33	1.89	7 (26%)
1	CFZ	B	57	1	18,21,22	2.52	7 (38%)	26,30,33	1.16	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	B	126	1	18,21,22	2.57	9 (50%)	26,30,33	2.01	7 (26%)
1	CFZ	B	440	1	18,21,22	2.50	7 (38%)	26,30,33	1.28	3 (11%)
1	UFT	B	13	1	18,21,22	2.58	9 (50%)	26,30,33	2.08	7 (26%)
1	CFZ	A	465	1	18,21,22	2.48	7 (38%)	26,30,33	1.30	2 (7%)
1	CFZ	B	298	1	18,21,22	2.53	7 (38%)	26,30,33	1.17	3 (11%)
1	UFT	A	460	1	18,21,22	2.61	9 (50%)	26,30,33	1.85	7 (26%)
1	CFZ	B	335	1	18,21,22	2.49	7 (38%)	26,30,33	1.36	2 (7%)
1	CFZ	B	620	1	18,21,22	2.48	7 (38%)	26,30,33	1.36	3 (11%)
1	CFZ	A	614	1	18,21,22	2.50	7 (38%)	26,30,33	1.20	3 (11%)
1	CFZ	B	679	1	18,21,22	2.49	7 (38%)	26,30,33	1.29	2 (7%)
1	UFT	B	358	1	18,21,22	2.64	9 (50%)	26,30,33	1.80	6 (23%)
1	UFT	A	135	1	18,21,22	2.63	9 (50%)	26,30,33	1.94	6 (23%)
1	UFT	B	14	1	18,21,22	2.60	9 (50%)	26,30,33	1.92	6 (23%)
1	UFT	A	126	1	18,21,22	2.58	9 (50%)	26,30,33	2.01	7 (26%)
1	UFT	B	270	1	18,21,22	2.57	10 (55%)	26,30,33	2.02	8 (30%)
1	UFT	B	217	1	18,21,22	2.61	10 (55%)	26,30,33	1.90	7 (26%)
1	UFT	B	499	1	18,21,22	2.62	9 (50%)	26,30,33	1.87	7 (26%)
1	UFT	B	500	1	18,21,22	2.56	10 (55%)	26,30,33	2.01	8 (30%)
1	CFZ	B	583	1	18,21,22	2.48	7 (38%)	26,30,33	1.48	4 (15%)
1	UFT	B	142	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	8 (30%)
1	UFT	B	61	1	18,21,22	2.59	9 (50%)	26,30,33	2.01	8 (30%)
1	UFT	B	92	1	18,21,22	2.61	10 (55%)	26,30,33	1.87	7 (26%)
1	UFT	B	143	1	18,21,22	2.57	9 (50%)	26,30,33	2.10	8 (30%)
1	CFZ	B	652	1	18,21,22	2.50	7 (38%)	26,30,33	1.22	3 (11%)
1	UFT	B	215	1	18,21,22	2.58	10 (55%)	26,30,33	1.97	8 (30%)
1	UFT	A	403	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	8 (30%)
1	UFT	A	524	1	18,21,22	2.68	9 (50%)	26,30,33	1.80	5 (19%)
1	UFT	A	190	1	18,21,22	2.58	10 (55%)	26,30,33	2.02	8 (30%)
1	CFZ	A	254	1	18,21,22	2.49	7 (38%)	26,30,33	1.21	3 (11%)
1	UFT	A	71	1	18,21,22	2.58	10 (55%)	26,30,33	1.99	7 (26%)
1	CFZ	B	417	1	18,21,22	2.49	7 (38%)	26,30,33	1.46	3 (11%)
1	CFZ	B	603	1	18,21,22	2.51	7 (38%)	26,30,33	1.20	3 (11%)
1	UFT	B	204	1	18,21,22	2.61	9 (50%)	26,30,33	1.89	6 (23%)
1	UFT	A	413	1	18,21,22	2.65	9 (50%)	26,30,33	1.80	6 (23%)
1	CFZ	B	139	1	18,21,22	2.49	7 (38%)	26,30,33	1.30	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CFZ	A	543	1	18,21,22	2.48	7 (38%)	26,30,33	1.31	4 (15%)
1	CFZ	B	700	1	18,21,22	2.51	7 (38%)	26,30,33	1.27	3 (11%)
1	CFZ	A	631	1	18,21,22	2.50	7 (38%)	26,30,33	1.35	3 (11%)
1	CFZ	A	332	1	18,21,22	2.49	7 (38%)	26,30,33	1.32	3 (11%)
1	CFZ	A	458	1	18,21,22	2.53	7 (38%)	26,30,33	1.25	2 (7%)
1	CFZ	B	610	1	18,21,22	2.48	7 (38%)	26,30,33	1.40	4 (15%)
1	UFT	A	377	1	18,21,22	2.62	9 (50%)	26,30,33	1.97	7 (26%)
1	UFT	A	489	1	18,21,22	2.58	9 (50%)	26,30,33	1.98	7 (26%)
1	CFZ	A	349	1	18,21,22	2.50	7 (38%)	26,30,33	1.19	3 (11%)
1	CFZ	A	664	1	18,21,22	2.47	7 (38%)	26,30,33	1.53	3 (11%)
1	CFZ	A	144	1	18,21,22	2.47	7 (38%)	26,30,33	1.52	3 (11%)
1	UFT	A	160	1	18,21,22	2.57	9 (50%)	26,30,33	1.99	8 (30%)
1	CFZ	B	157	1	18,21,22	2.51	7 (38%)	26,30,33	1.17	2 (7%)
1	CFZ	A	536	1	18,21,22	2.48	7 (38%)	26,30,33	1.50	2 (7%)
1	UFT	B	105	1	18,21,22	2.59	9 (50%)	26,30,33	1.95	7 (26%)
1	UFT	A	245	1	18,21,22	2.59	9 (50%)	26,30,33	1.94	8 (30%)
1	UFT	A	593	1	18,21,22	2.59	9 (50%)	26,30,33	1.95	8 (30%)
1	CFZ	A	157	1	18,21,22	2.51	7 (38%)	26,30,33	1.16	2 (7%)
1	UFT	B	663	1	18,21,22	2.56	10 (55%)	26,30,33	2.08	8 (30%)
1	UFT	B	137	1	18,21,22	2.59	9 (50%)	26,30,33	1.90	8 (30%)
1	UFT	A	98	1	18,21,22	2.60	10 (55%)	26,30,33	1.93	7 (26%)
1	UFT	A	301	1	18,21,22	2.57	9 (50%)	26,30,33	1.98	8 (30%)
1	UFT	B	50	1	18,21,22	2.58	9 (50%)	26,30,33	2.05	6 (23%)
1	UFT	A	101	1	18,21,22	2.57	10 (55%)	26,30,33	2.06	8 (30%)
1	CFZ	A	246	1	18,21,22	2.51	7 (38%)	26,30,33	1.19	3 (11%)
1	CFZ	A	639	1	18,21,22	2.49	7 (38%)	26,30,33	1.29	3 (11%)
1	UFT	A	153	1	18,21,22	2.63	9 (50%)	26,30,33	1.88	7 (26%)
1	UFT	B	19	1	18,21,22	2.59	9 (50%)	26,30,33	1.96	8 (30%)
1	UFT	A	62	1	18,21,22	2.56	10 (55%)	26,30,33	2.07	8 (30%)
1	CFZ	B	308	1	18,21,22	2.47	7 (38%)	26,30,33	1.51	4 (15%)
1	UFT	A	55	1	18,21,22	2.61	9 (50%)	26,30,33	1.89	7 (26%)
1	CFZ	A	247	1	18,21,22	2.50	7 (38%)	26,30,33	1.17	2 (7%)
1	CFZ	B	625	1	18,21,22	2.48	7 (38%)	26,30,33	1.33	3 (11%)
1	CFZ	A	632	1	18,21,22	2.49	7 (38%)	26,30,33	1.26	2 (7%)
1	CFZ	A	75	1	18,21,22	2.45	7 (38%)	26,30,33	1.46	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UFT	A	701	1	18,21,22	2.59	9 (50%)	26,30,33	1.98	7 (26%)
1	CFZ	A	298	1	18,21,22	2.53	7 (38%)	26,30,33	1.18	3 (11%)
1	CFZ	A	110	1	18,21,22	2.50	7 (38%)	26,30,33	1.21	3 (11%)
1	CFZ	B	643	1	18,21,22	2.51	7 (38%)	26,30,33	1.24	3 (11%)
1	CFZ	B	173	1	18,21,22	2.49	7 (38%)	26,30,33	1.20	2 (7%)
1	CFZ	A	173	1	18,21,22	2.49	7 (38%)	26,30,33	1.18	2 (7%)
1	CFZ	B	486	1	18,21,22	2.48	7 (38%)	26,30,33	1.29	2 (7%)
1	CFZ	B	249	1	18,21,22	2.51	7 (38%)	26,30,33	1.19	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	B	155	1	-	0/7/25/26	0/2/2/2
1	UFT	A	530	1	-	2/7/25/26	0/2/2/2
1	UFT	A	143	1	-	2/7/25/26	0/2/2/2
1	UFT	A	200	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	446	1	-	0/7/25/26	0/2/2/2
1	UFT	B	504	1	-	2/7/25/26	0/2/2/2
1	UFT	A	358	1	-	0/7/25/26	0/2/2/2
1	UFT	B	402	1	-	0/7/25/26	0/2/2/2
1	UFT	B	695	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	328	1	-	3/7/25/26	0/2/2/2
1	UFT	B	42	1	-	0/7/25/26	0/2/2/2
1	UFT	A	662	1	-	2/7/25/26	0/2/2/2
1	UFT	A	542	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	407	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	458	1	-	0/7/25/26	0/2/2/2
1	UFT	A	115	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	372	1	-	0/7/25/26	0/2/2/2
1	UFT	A	559	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	540	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	10	1	-	2/7/25/26	0/2/2/2
1	UFT	A	322	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	111	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	477	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	198	1	-	0/7/25/26	0/2/2/2
1	UFT	B	116	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	643	1	-	0/7/25/26	0/2/2/2
1	UFT	A	233	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	372	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	241	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	438	1	-	0/7/25/26	0/2/2/2
1	UFT	A	367	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	564	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	462	1	-	0/7/25/26	0/2/2/2
1	UFT	A	251	1	-	2/7/25/26	0/2/2/2
1	UFT	A	636	1	-	0/7/25/26	0/2/2/2
1	UFT	B	509	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	564	1	-	3/7/25/26	0/2/2/2
1	UFT	A	545	1	-	3/7/25/26	0/2/2/2
1	UFT	B	690	1	-	0/7/25/26	0/2/2/2
1	UFT	B	59	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	558	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	90	1	-	0/7/25/26	0/2/2/2
1	UFT	A	142	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	219	1	-	2/7/25/26	0/2/2/2
1	UFT	A	493	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	548	1	-	1/7/25/26	0/2/2/2
1	UFT	A	513	1	-	2/7/25/26	0/2/2/2
1	UFT	B	293	1	-	2/7/25/26	0/2/2/2
1	UFT	A	42	1	-	0/7/25/26	0/2/2/2
1	UFT	B	549	1	-	2/7/25/26	0/2/2/2
1	UFT	B	719	1	-	2/7/25/26	0/2/2/2
1	UFT	B	684	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	308	1	-	0/7/25/26	0/2/2/2
1	UFT	B	618	1	-	0/7/25/26	0/2/2/2
1	UFT	B	202	1	-	2/7/25/26	0/2/2/2
1	UFT	A	215	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	210	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	405	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	67	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	455	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	90	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	164	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	417	1	-	0/7/25/26	0/2/2/2
1	UFT	A	689	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	25	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	411	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	614	1	-	2/7/25/26	0/2/2/2
1	UFT	B	485	1	-	2/7/25/26	0/2/2/2
1	UFT	A	74	1	-	2/7/25/26	0/2/2/2
1	UFT	A	635	1	-	1/7/25/26	0/2/2/2
1	UFT	B	141	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	667	1	-	2/7/25/26	0/2/2/2
1	UFT	A	347	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	268	1	-	0/7/25/26	0/2/2/2
1	UFT	A	366	1	-	0/7/25/26	0/2/2/2
1	UFT	B	302	1	-	2/7/25/26	0/2/2/2
1	UFT	B	94	1	-	1/7/25/26	0/2/2/2
1	UFT	B	635	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	556	1	-	6/7/25/26	0/2/2/2
1	UFT	B	365	1	-	0/7/25/26	0/2/2/2
1	UFT	B	309	1	-	2/7/25/26	0/2/2/2
1	UFT	B	313	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	76	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	316	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	79	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	114	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	151	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	604	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	165	1	-	0/7/25/26	0/2/2/2
1	UFT	A	695	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	576	1	-	0/7/25/26	0/2/2/2
1	UFT	A	88	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	21	1	-	0/7/25/26	0/2/2/2
1	UFT	A	633	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	21	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	404	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	242	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	565	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	355	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	174	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	387	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	604	1	-	0/7/25/26	0/2/2/2
1	UFT	B	175	1	-	2/7/25/26	0/2/2/2
1	UFT	B	628	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	498	1	-	0/7/25/26	0/2/2/2
1	UFT	B	489	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	664	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	651	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	206	1	-	2/7/25/26	0/2/2/2
1	UFT	B	11	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	518	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	161	1	-	0/7/25/26	0/2/2/2
1	UFT	A	229	1	-	3/7/25/26	0/2/2/2
1	UFT	A	663	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	246	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	25	1	-	3/7/25/26	0/2/2/2
1	UFT	B	182	1	-	0/7/25/26	0/2/2/2
1	UFT	B	154	1	-	0/7/25/26	0/2/2/2
1	UFT	B	44	1	-	2/7/25/26	0/2/2/2
1	UFT	B	431	1	-	2/7/25/26	0/2/2/2
1	UFT	B	602	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	373	1	-	0/7/25/26	0/2/2/2
1	UFT	B	344	1	-	2/7/25/26	0/2/2/2
1	UFT	B	447	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	540	1	-	2/7/25/26	0/2/2/2
1	UFT	A	169	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	117	1	-	2/7/25/26	0/2/2/2
1	UFT	B	701	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	110	1	-	2/7/25/26	0/2/2/2
1	UFT	B	170	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	201	1	-	2/7/25/26	0/2/2/2
1	UFT	B	554	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	103	1	-	0/7/25/26	0/2/2/2
1	UFT	B	106	1	-	3/7/25/26	0/2/2/2
1	UFT	B	153	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	603	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	439	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	469	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	381	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	523	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	637	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	184	1	-	2/7/25/26	0/2/2/2
1	UFT	A	609	1	-	0/7/25/26	0/2/2/2
1	UFT	A	669	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	353	1	-	0/7/25/26	0/2/2/2
1	UFT	A	196	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	285	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	363	1	-	2/7/25/26	0/2/2/2
1	UFT	A	155	1	-	0/7/25/26	0/2/2/2
1	UFT	B	334	1	-	3/7/25/26	0/2/2/2
1	UFT	A	216	1	-	0/7/25/26	0/2/2/2
1	UFT	A	84	1	-	3/7/25/26	0/2/2/2
1	UFT	B	571	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	439	1	-	0/7/25/26	0/2/2/2
1	UFT	B	80	1	-	2/7/25/26	0/2/2/2
1	UFT	B	662	1	-	2/7/25/26	0/2/2/2
1	UFT	B	456	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	96	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	406	1	-	2/7/25/26	0/2/2/2
1	UFT	A	329	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	325	1	-	2/7/25/26	0/2/2/2
1	UFT	A	163	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	369	1	-	0/7/25/26	0/2/2/2
1	UFT	B	621	1	-	3/7/25/26	0/2/2/2
1	UFT	B	524	1	-	3/7/25/26	0/2/2/2
1	UFT	B	472	1	-	3/7/25/26	0/2/2/2
1	UFT	B	245	1	-	0/7/25/26	0/2/2/2
1	UFT	B	84	1	-	3/7/25/26	0/2/2/2
1	UFT	B	607	1	-	2/7/25/26	0/2/2/2
1	UFT	B	305	1	-	2/7/25/26	0/2/2/2
1	UFT	B	229	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	600	1	-	0/7/25/26	0/2/2/2
1	UFT	A	214	1	-	0/7/25/26	0/2/2/2
1	UFT	B	555	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	418	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	698	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	679	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	506	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	486	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	378	1	-	0/7/25/26	0/2/2/2
1	UFT	A	690	1	-	0/7/25/26	0/2/2/2
1	UFT	A	504	1	-	2/7/25/26	0/2/2/2
1	UFT	B	60	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	362	1	-	0/7/25/26	0/2/2/2
1	UFT	A	265	1	-	0/7/25/26	0/2/2/2
1	UFT	A	204	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	704	1	-	2/7/25/26	0/2/2/2
1	UFT	A	430	1	-	0/7/25/26	0/2/2/2
1	UFT	B	535	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	647	1	-	0/7/25/26	0/2/2/2
1	UFT	A	581	1	-	0/7/25/26	0/2/2/2
1	UFT	B	636	1	-	0/7/25/26	0/2/2/2
1	UFT	A	309	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	518	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	404	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	104	1	-	0/7/25/26	0/2/2/2
1	UFT	A	296	1	-	2/7/25/26	0/2/2/2
1	UFT	A	179	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	576	1	-	0/7/25/26	0/2/2/2
1	UFT	A	33	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	218	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	156	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	551	1	-	0/7/25/26	0/2/2/2
1	UFT	B	71	1	-	0/7/25/26	0/2/2/2
1	UFT	A	202	1	-	1/7/25/26	0/2/2/2
1	UFT	A	86	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	543	1	-	0/7/25/26	0/2/2/2
1	UFT	A	8	1	-	0/7/25/26	0/2/2/2
1	UFT	A	555	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	383	1	-	2/7/25/26	0/2/2/2
1	UFT	A	471	1	-	2/7/25/26	0/2/2/2
1	UFT	A	14	1	-	0/7/25/26	0/2/2/2
1	UFT	A	481	1	-	2/7/25/26	0/2/2/2
1	UFT	A	582	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	592	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	323	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	370	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	28	1	-	2/7/25/26	0/2/2/2
1	UFT	B	687	1	-	0/7/25/26	0/2/2/2
1	UFT	A	141	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	315	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	39	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	72	1	-	0/7/25/26	0/2/2/2
1	UFT	B	361	1	-	2/7/25/26	0/2/2/2
1	UFT	A	673	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	140	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	494	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	131	1	-	0/7/25/26	0/2/2/2
1	UFT	A	302	1	-	2/7/25/26	0/2/2/2
1	UFT	B	466	1	-	0/7/25/26	0/2/2/2
1	UFT	B	437	1	-	0/7/25/26	0/2/2/2
1	UFT	B	629	1	-	0/7/25/26	0/2/2/2
1	UFT	A	621	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	354	1	-	2/7/25/26	0/2/2/2
1	UFT	B	544	1	-	2/7/25/26	0/2/2/2
1	UFT	A	313	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	76	1	-	2/7/25/26	0/2/2/2
1	UFT	A	350	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	425	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	120	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	67	1	-	2/7/25/26	0/2/2/2
1	UFT	A	359	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	335	1	-	2/7/25/26	0/2/2/2
1	UFT	A	549	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	652	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	657	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	451	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	130	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	151	1	-	2/7/25/26	0/2/2/2
1	UFT	A	97	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	57	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	438	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	492	1	-	0/7/25/26	0/2/2/2
1	UFT	B	581	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	579	1	-	0/7/25/26	0/2/2/2
1	UFT	A	719	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	693	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	583	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	338	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	585	1	-	0/7/25/26	0/2/2/2
1	UFT	B	669	1	-	2/7/25/26	0/2/2/2
1	UFT	A	112	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	117	1	-	2/7/25/26	0/2/2/2
1	UFT	B	179	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	370	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	285	1	-	0/7/25/26	0/2/2/2
1	UFT	B	689	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	338	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	279	1	-	0/7/25/26	0/2/2/2
1	UFT	B	666	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	171	1	-	2/7/25/26	0/2/2/2
1	UFT	B	174	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	282	1	-	0/7/25/26	0/2/2/2
1	UFT	A	260	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	528	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	637	1	-	2/7/25/26	0/2/2/2
1	UFT	B	169	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	625	1	-	1/7/25/26	0/2/2/2
1	UFT	A	608	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	655	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	600	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	140	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	131	1	-	0/7/25/26	0/2/2/2
1	UFT	B	377	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	517	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	63	1	-	2/7/25/26	0/2/2/2
1	UFT	B	197	1	-	0/7/25/26	0/2/2/2
1	UFT	B	135	1	-	0/7/25/26	0/2/2/2
1	UFT	A	500	1	-	0/7/25/26	0/2/2/2
1	UFT	B	74	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	426	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	418	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	316	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	492	1	-	0/7/25/26	0/2/2/2
1	UFT	A	653	1	-	0/7/25/26	0/2/2/2
1	UFT	B	389	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	156	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	498	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	399	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	667	1	-	2/7/25/26	0/2/2/2
1	UFT	B	423	1	-	2/7/25/26	0/2/2/2
1	UFT	B	606	1	-	0/7/25/26	0/2/2/2
1	UFT	B	633	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	473	1	-	2/7/25/26	0/2/2/2
1	UFT	A	703	1	-	2/7/25/26	0/2/2/2
1	UFT	B	398	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	459	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	585	1	-	0/7/25/26	0/2/2/2
1	UFT	A	554	1	-	0/7/25/26	0/2/2/2
1	UFT	A	434	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	49	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	325	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	511	1	-	0/7/25/26	0/2/2/2
1	UFT	A	105	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	351	1	-	2/7/25/26	0/2/2/2
1	UFT	B	108	1	-	2/7/25/26	0/2/2/2
1	UFT	B	421	1	-	0/7/25/26	0/2/2/2
1	UFT	A	687	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	444	1	-	0/7/25/26	0/2/2/2
1	UFT	A	629	1	-	0/7/25/26	0/2/2/2
1	UFT	A	447	1	-	0/7/25/26	0/2/2/2
1	UFT	B	214	1	-	0/7/25/26	0/2/2/2
1	UFT	B	464	1	-	2/7/25/26	0/2/2/2
1	UFT	B	352	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	407	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	315	1	-	0/7/25/26	0/2/2/2
1	UFT	A	402	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	130	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	491	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	B	266	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	15	1	-	3/7/25/26	0/2/2/2
1	UFT	B	673	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	446	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	424	1	-	1/7/25/26	0/2/2/2
1	UFT	A	503	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	592	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	512	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	209	1	-	0/7/25/26	0/2/2/2
1	UFT	A	208	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	440	1	-	2/7/25/26	0/2/2/2
1	UFT	B	43	1	-	4/7/25/26	0/2/2/2
1	UFT	B	32	1	-	2/7/25/26	0/2/2/2
1	UFT	B	703	1	-	2/7/25/26	0/2/2/2
1	UFT	B	33	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	232	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	234	1	-	3/7/25/26	0/2/2/2
1	UFT	A	32	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	459	1	-	0/7/25/26	0/2/2/2
1	UFT	A	676	1	-	3/7/25/26	0/2/2/2
1	UFT	A	712	1	-	2/7/25/26	0/2/2/2
1	UFT	A	108	1	-	2/7/25/26	0/2/2/2
1	UFT	A	646	1	-	0/7/25/26	0/2/2/2
1	UFT	B	430	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	129	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	247	1	-	0/7/25/26	0/2/2/2
1	UFT	A	344	1	-	3/7/25/26	0/2/2/2
1	UFT	A	19	1	-	2/7/25/26	0/2/2/2
1	UFT	A	50	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	378	1	-	0/7/25/26	0/2/2/2
1	UFT	B	471	1	-	0/7/25/26	0/2/2/2
1	UFT	B	481	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	384	1	-	0/7/25/26	0/2/2/2
1	UFT	A	684	1	-	2/7/25/26	0/2/2/2
1	UFT	A	659	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	241	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	321	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	568	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	631	1	-	0/7/25/26	0/2/2/2
1	UFT	B	542	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	321	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	587	1	-	2/7/25/26	0/2/2/2
1	UFT	A	217	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	568	1	-	0/7/25/26	0/2/2/2
1	UFT	A	398	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	234	1	-	3/7/25/26	0/2/2/2
1	UFT	B	190	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	536	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	647	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	639	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	587	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	73	1	-	0/7/25/26	0/2/2/2
1	UFT	B	359	1	-	0/7/25/26	0/2/2/2
1	UFT	B	283	1	-	2/7/25/26	0/2/2/2
1	UFT	B	366	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	426	1	-	0/7/25/26	0/2/2/2
1	UFT	B	534	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	657	1	-	2/7/25/26	0/2/2/2
1	UFT	B	55	1	-	0/7/25/26	0/2/2/2
1	UFT	A	192	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	120	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	124	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	682	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	383	1	-	0/7/25/26	0/2/2/2
1	UFT	A	618	1	-	0/7/25/26	0/2/2/2
1	UFT	A	666	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	579	1	-	0/7/25/26	0/2/2/2
1	UFT	A	293	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	441	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	328	1	-	3/7/25/26	0/2/2/2
1	UFT	A	628	1	-	0/7/25/26	0/2/2/2
1	UFT	A	137	1	-	0/7/25/26	0/2/2/2
1	UFT	B	98	1	-	0/7/25/26	0/2/2/2
1	UFT	B	301	1	-	2/7/25/26	0/2/2/2
1	UFT	A	485	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	548	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	399	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	332	1	-	2/7/25/26	0/2/2/2
1	UFT	B	530	1	-	2/7/25/26	0/2/2/2
1	UFT	B	656	1	-	0/7/25/26	0/2/2/2
1	UFT	B	48	1	-	0/7/25/26	0/2/2/2
1	UFT	A	44	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	282	1	-	0/7/25/26	0/2/2/2
1	UFT	B	296	1	-	2/7/25/26	0/2/2/2
1	UFT	A	89	1	-	0/7/25/26	0/2/2/2
1	UFT	A	544	1	-	2/7/25/26	0/2/2/2
1	UFT	A	11	1	-	0/7/25/26	0/2/2/2
1	UFT	B	593	1	-	3/7/25/26	0/2/2/2
1	UFT	A	352	1	-	2/7/25/26	0/2/2/2
1	UFT	B	712	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	46	1	-	2/7/25/26	0/2/2/2
1	UFT	A	432	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	565	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	655	1	-	2/7/25/26	0/2/2/2
1	UFT	A	365	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	304	1	-	0/7/25/26	0/2/2/2
1	UFT	A	431	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	124	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	79	1	-	0/7/25/26	0/2/2/2
1	UFT	B	200	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	198	1	-	0/7/25/26	0/2/2/2
1	UFT	A	43	1	-	4/7/25/26	0/2/2/2
1	CFZ	A	474	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	75	1	-	1/7/25/26	0/2/2/2
1	UFT	B	347	1	-	2/7/25/26	0/2/2/2
1	UFT	A	182	1	-	0/7/25/26	0/2/2/2
1	UFT	B	653	1	-	0/7/25/26	0/2/2/2
1	UFT	B	367	1	-	2/7/25/26	0/2/2/2
1	UFT	B	590	1	-	1/7/25/26	0/2/2/2
1	UFT	B	251	1	-	2/7/25/26	0/2/2/2
1	UFT	A	175	1	-	2/7/25/26	0/2/2/2
1	UFT	B	322	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	26	1	-	1/7/25/26	0/2/2/2
1	UFT	A	334	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	691	1	-	0/7/25/26	0/2/2/2
1	UFT	B	493	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	210	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	184	1	-	2/7/25/26	0/2/2/2
1	UFT	A	456	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	49	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	436	1	-	0/7/25/26	0/2/2/2
1	UFT	B	577	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	411	1	-	0/7/25/26	0/2/2/2
1	UFT	B	708	1	-	0/7/25/26	0/2/2/2
1	UFT	B	196	1	-	3/7/25/26	0/2/2/2
1	UFT	A	696	1	-	0/7/25/26	0/2/2/2
1	UFT	A	472	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	279	1	-	0/7/25/26	0/2/2/2
1	UFT	A	116	1	-	0/7/25/26	0/2/2/2
1	UFT	B	115	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	242	1	-	0/7/25/26	0/2/2/2
1	UFT	B	336	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	556	1	-	6/7/25/26	0/2/2/2
1	UFT	B	86	1	-	0/7/25/26	0/2/2/2
1	UFT	A	336	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	382	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	171	1	-	2/7/25/26	0/2/2/2
1	UFT	B	502	1	-	2/7/25/26	0/2/2/2
1	UFT	B	545	1	-	3/7/25/26	0/2/2/2
1	UFT	B	163	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	698	1	-	0/7/25/26	0/2/2/2
1	UFT	A	59	1	-	0/7/25/26	0/2/2/2
1	UFT	A	170	1	-	1/7/25/26	0/2/2/2
1	UFT	A	283	1	-	2/7/25/26	0/2/2/2
1	UFT	B	89	1	-	0/7/25/26	0/2/2/2
1	UFT	B	432	1	-	1/7/25/26	0/2/2/2
1	UFT	A	270	1	-	2/7/25/26	0/2/2/2
1	UFT	A	197	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	63	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	15	1	-	2/7/25/26	0/2/2/2
1	UFT	B	62	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	212	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	360	1	-	2/7/25/26	0/2/2/2
1	UFT	A	606	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	188	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	363	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	212	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	425	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	351	1	-	0/7/25/26	0/2/2/2
1	UFT	B	97	1	-	3/7/25/26	0/2/2/2
1	UFT	B	265	1	-	0/7/25/26	0/2/2/2
1	UFT	A	656	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	218	1	-	0/7/25/26	0/2/2/2
1	UFT	B	646	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	34	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	381	1	-	1/7/25/26	0/2/2/2
1	UFT	B	434	1	-	0/7/25/26	0/2/2/2
1	UFT	A	602	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	693	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	355	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	405	1	-	2/7/25/26	0/2/2/2
1	UFT	A	60	1	-	0/7/25/26	0/2/2/2
1	UFT	A	464	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	384	1	-	3/7/25/26	0/2/2/2
1	UFT	A	13	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	268	1	-	0/7/25/26	0/2/2/2
1	UFT	B	329	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	373	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	72	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	206	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	506	1	-	2/7/25/26	0/2/2/2
1	UFT	B	582	1	-	2/7/25/26	0/2/2/2
1	UFT	B	233	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	232	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	149	1	-	0/7/25/26	0/2/2/2
1	UFT	A	61	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	165	1	-	0/7/25/26	0/2/2/2
1	UFT	A	389	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	354	1	-	1/7/25/26	0/2/2/2
1	UFT	A	266	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	499	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	103	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	104	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	682	1	-	0/7/25/26	0/2/2/2
1	UFT	A	571	1	-	2/7/25/26	0/2/2/2
1	UFT	B	88	1	-	2/7/25/26	0/2/2/2
1	UFT	B	609	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	651	1	-	0/7/25/26	0/2/2/2
1	UFT	A	361	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	465	1	-	0/7/25/26	0/2/2/2
1	UFT	B	69	1	-	0/7/25/26	0/2/2/2
1	UFT	B	676	1	-	3/7/25/26	0/2/2/2
1	UFT	A	154	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	26	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	491	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	610	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	323	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	201	1	-	2/7/25/26	0/2/2/2
1	UFT	B	513	1	-	1/7/25/26	0/2/2/2
1	UFT	A	577	1	-	0/7/25/26	0/2/2/2
1	UFT	B	659	1	-	3/7/25/26	0/2/2/2
1	UFT	A	305	1	-	2/7/25/26	0/2/2/2
1	UFT	A	466	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	111	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	96	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	39	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	369	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	512	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	704	1	-	2/7/25/26	0/2/2/2
1	UFT	B	559	1	-	1/7/25/26	0/2/2/2
1	UFT	B	519	1	-	2/7/25/26	0/2/2/2
1	UFT	A	92	1	-	2/7/25/26	0/2/2/2
1	UFT	A	106	1	-	3/7/25/26	0/2/2/2
1	CFZ	B	304	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	360	1	-	0/7/25/26	0/2/2/2
1	UFT	A	437	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	469	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	523	1	-	1/7/25/26	0/2/2/2
1	UFT	B	260	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	558	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	474	1	-	2/7/25/26	0/2/2/2
1	UFT	B	208	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	46	1	-	2/7/25/26	0/2/2/2
1	UFT	B	608	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	700	1	-	2/7/25/26	0/2/2/2
1	UFT	B	192	1	-	3/7/25/26	0/2/2/2
1	UFT	A	69	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	424	1	-	1/7/25/26	0/2/2/2
1	UFT	A	423	1	-	2/7/25/26	0/2/2/2
1	UFT	B	460	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	517	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	249	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	406	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	149	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	528	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	550	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	353	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	691	1	-	0/7/25/26	0/2/2/2
1	UFT	A	502	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	550	1	-	0/7/25/26	0/2/2/2
1	UFT	B	216	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	161	1	-	0/7/25/26	0/2/2/2
1	UFT	A	607	1	-	2/7/25/26	0/2/2/2
1	UFT	B	403	1	-	0/7/25/26	0/2/2/2
1	UFT	A	80	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	362	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	254	1	-	0/7/25/26	0/2/2/2
1	UFT	B	112	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	34	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	551	1	-	0/7/25/26	0/2/2/2
1	UFT	B	696	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	473	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	144	1	-	2/7/25/26	0/2/2/2
1	UFT	A	509	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	477	1	-	3/7/25/26	0/2/2/2
1	UFT	A	534	1	-	2/7/25/26	0/2/2/2
1	UFT	A	535	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	B	8	1	-	2/7/25/26	0/2/2/2
1	UFT	B	101	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	28	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	574	1	-	0/7/25/26	0/2/2/2
1	UFT	B	160	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	387	1	-	2/7/25/26	0/2/2/2
1	UFT	B	720	1	1/1/5/5	3/7/25/26	0/2/2/2
1	CFZ	A	209	1	-	0/7/25/26	0/2/2/2
1	UFT	A	708	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	441	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	188	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	494	1	-	0/7/25/26	0/2/2/2
1	UFT	A	48	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	219	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	114	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	73	1	-	0/7/25/26	0/2/2/2
1	UFT	A	590	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	164	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	574	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	632	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	139	1	-	0/7/25/26	0/2/2/2
1	UFT	A	519	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	511	1	-	0/7/25/26	0/2/2/2
1	UFT	A	94	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	620	1	-	0/7/25/26	0/2/2/2
1	UFT	A	720	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	10	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	129	1	-	0/7/25/26	0/2/2/2
1	UFT	A	421	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	57	1	-	2/7/25/26	0/2/2/2
1	UFT	B	126	1	-	1/7/25/26	0/2/2/2
1	CFZ	B	440	1	-	1/7/25/26	0/2/2/2
1	UFT	B	13	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	465	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	298	1	-	2/7/25/26	0/2/2/2
1	UFT	A	460	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	335	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	620	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	614	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	B	679	1	-	0/7/25/26	0/2/2/2
1	UFT	B	358	1	-	0/7/25/26	0/2/2/2
1	UFT	A	135	1	-	0/7/25/26	0/2/2/2
1	UFT	B	14	1	-	0/7/25/26	0/2/2/2
1	UFT	A	126	1	-	1/7/25/26	0/2/2/2
1	UFT	B	270	1	-	2/7/25/26	0/2/2/2
1	UFT	B	217	1	-	0/7/25/26	0/2/2/2
1	UFT	B	499	1	-	3/7/25/26	0/2/2/2
1	UFT	B	500	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	583	1	-	2/7/25/26	0/2/2/2
1	UFT	B	142	1	-	0/7/25/26	0/2/2/2
1	UFT	B	61	1	-	2/7/25/26	0/2/2/2
1	UFT	B	92	1	-	2/7/25/26	0/2/2/2
1	UFT	B	143	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	652	1	-	0/7/25/26	0/2/2/2
1	UFT	B	215	1	-	0/7/25/26	0/2/2/2
1	UFT	A	403	1	-	0/7/25/26	0/2/2/2
1	UFT	A	524	1	-	0/7/25/26	0/2/2/2
1	UFT	A	190	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	254	1	-	0/7/25/26	0/2/2/2
1	UFT	A	71	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	417	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	603	1	-	0/7/25/26	0/2/2/2
1	UFT	B	204	1	-	0/7/25/26	0/2/2/2
1	UFT	A	413	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	139	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	543	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	700	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	631	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	332	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	458	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	610	1	-	1/7/25/26	0/2/2/2
1	UFT	A	377	1	-	3/7/25/26	0/2/2/2
1	UFT	A	489	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	349	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	664	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	144	1	-	2/7/25/26	0/2/2/2
1	UFT	A	160	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	157	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	536	1	-	0/7/25/26	0/2/2/2
1	UFT	B	105	1	-	1/7/25/26	0/2/2/2
1	UFT	A	245	1	-	0/7/25/26	0/2/2/2
1	UFT	A	593	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	157	1	-	0/7/25/26	0/2/2/2
1	UFT	B	663	1	-	0/7/25/26	0/2/2/2
1	UFT	B	137	1	-	0/7/25/26	0/2/2/2
1	UFT	A	98	1	-	0/7/25/26	0/2/2/2
1	UFT	A	301	1	-	2/7/25/26	0/2/2/2
1	UFT	B	50	1	-	1/7/25/26	0/2/2/2
1	UFT	A	101	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	246	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	639	1	-	2/7/25/26	0/2/2/2
1	UFT	A	153	1	-	0/7/25/26	0/2/2/2
1	UFT	B	19	1	-	2/7/25/26	0/2/2/2
1	UFT	A	62	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	308	1	-	0/7/25/26	0/2/2/2
1	UFT	A	55	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	247	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	625	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	632	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	75	1	-	2/7/25/26	0/2/2/2
1	UFT	A	701	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	298	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	110	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	643	1	-	0/7/25/26	0/2/2/2
1	CFZ	B	173	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	173	1	-	2/7/25/26	0/2/2/2
1	CFZ	B	486	1	-	4/7/25/26	0/2/2/2
1	CFZ	B	249	1	-	0/7/25/26	0/2/2/2

All (5758) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	493	UFT	C2-N1	5.30	1.47	1.38
1	A	359	UFT	C2-N1	5.22	1.46	1.38
1	B	105	UFT	C2-N1	5.17	1.46	1.38
1	A	43	UFT	C2-N1	5.16	1.46	1.38
1	B	43	UFT	C2-N1	5.14	1.46	1.38
1	B	42	UFT	C2-N1	5.13	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	UFT	C2-N1	5.10	1.46	1.38
1	A	358	UFT	C2-N1	5.10	1.46	1.38
1	A	105	UFT	C2-N1	5.10	1.46	1.38
1	A	216	UFT	C2-N1	5.09	1.46	1.38
1	A	524	UFT	C2-N1	5.09	1.46	1.38
1	B	523	CFZ	C4-N4	5.02	1.45	1.33
1	A	322	UFT	C2-N1	5.02	1.46	1.38
1	B	358	UFT	C2-N1	5.01	1.46	1.38
1	B	676	UFT	C2-N1	5.00	1.46	1.38
1	B	491	CFZ	C4-N4	5.00	1.45	1.33
1	A	676	UFT	C2-N1	4.99	1.46	1.38
1	B	513	UFT	C2-N1	4.98	1.46	1.38
1	B	282	CFZ	C4-N4	4.98	1.45	1.33
1	B	404	CFZ	C4-N4	4.98	1.45	1.33
1	B	210	CFZ	C4-N4	4.98	1.45	1.33
1	A	579	CFZ	C4-N4	4.98	1.45	1.33
1	A	446	CFZ	C4-N4	4.98	1.45	1.33
1	B	268	CFZ	C4-N4	4.97	1.45	1.33
1	B	407	CFZ	C4-N4	4.97	1.45	1.33
1	A	323	CFZ	C4-N4	4.97	1.45	1.33
1	A	383	CFZ	C4-N4	4.97	1.45	1.33
1	B	657	CFZ	C4-N4	4.97	1.45	1.33
1	A	360	CFZ	C4-N4	4.97	1.45	1.33
1	B	486	CFZ	C4-N4	4.97	1.45	1.33
1	A	637	CFZ	C4-N4	4.97	1.45	1.33
1	A	512	CFZ	C4-N4	4.97	1.45	1.33
1	B	587	CFZ	C4-N4	4.97	1.45	1.33
1	A	474	CFZ	C4-N4	4.97	1.45	1.33
1	A	491	CFZ	C4-N4	4.97	1.45	1.33
1	A	103	CFZ	C4-N4	4.97	1.45	1.33
1	B	383	CFZ	C4-N4	4.97	1.45	1.33
1	B	381	CFZ	C4-N4	4.97	1.45	1.33
1	A	254	CFZ	C4-N4	4.97	1.45	1.33
1	B	76	CFZ	C4-N4	4.97	1.45	1.33
1	A	184	CFZ	C4-N4	4.97	1.45	1.33
1	B	384	CFZ	C4-N4	4.97	1.45	1.33
1	A	417	CFZ	C4-N4	4.97	1.45	1.33
1	B	700	CFZ	C4-N4	4.97	1.45	1.33
1	A	528	CFZ	C4-N4	4.97	1.45	1.33
1	A	79	CFZ	C4-N4	4.97	1.45	1.33
1	B	558	CFZ	C4-N4	4.96	1.45	1.33
1	A	620	CFZ	C4-N4	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	CFZ	C4-N4	4.96	1.45	1.33
1	A	698	CFZ	C4-N4	4.96	1.45	1.33
1	A	315	CFZ	C4-N4	4.96	1.45	1.33
1	B	369	CFZ	C4-N4	4.96	1.45	1.33
1	B	652	CFZ	C4-N4	4.96	1.45	1.33
1	B	363	CFZ	C4-N4	4.96	1.45	1.33
1	A	564	CFZ	C4-N4	4.96	1.45	1.33
1	A	600	CFZ	C4-N4	4.96	1.45	1.33
1	B	691	CFZ	C4-N4	4.96	1.45	1.33
1	A	405	CFZ	C4-N4	4.96	1.45	1.33
1	A	28	CFZ	C4-N4	4.96	1.45	1.33
1	B	304	CFZ	C4-N4	4.96	1.45	1.33
1	A	426	CFZ	C4-N4	4.96	1.45	1.33
1	A	67	CFZ	C4-N4	4.96	1.45	1.33
1	A	72	CFZ	C4-N4	4.96	1.45	1.33
1	A	328	CFZ	C4-N4	4.96	1.45	1.33
1	A	373	CFZ	C4-N4	4.96	1.45	1.33
1	A	304	CFZ	C4-N4	4.96	1.45	1.33
1	A	140	CFZ	C4-N4	4.96	1.45	1.33
1	B	355	CFZ	C4-N4	4.96	1.45	1.33
1	B	579	CFZ	C4-N4	4.96	1.45	1.33
1	A	268	CFZ	C4-N4	4.96	1.45	1.33
1	B	161	CFZ	C4-N4	4.96	1.45	1.33
1	A	643	CFZ	C4-N4	4.96	1.45	1.33
1	A	667	CFZ	C4-N4	4.96	1.45	1.33
1	A	165	CFZ	C4-N4	4.96	1.45	1.33
1	B	446	CFZ	C4-N4	4.96	1.45	1.33
1	A	465	CFZ	C4-N4	4.96	1.45	1.33
1	B	465	CFZ	C4-N4	4.96	1.45	1.33
1	B	614	CFZ	C4-N4	4.96	1.45	1.33
1	A	39	CFZ	C4-N4	4.96	1.45	1.33
1	B	212	CFZ	C4-N4	4.96	1.45	1.33
1	A	110	CFZ	C4-N4	4.96	1.45	1.33
1	A	657	CFZ	C4-N4	4.96	1.45	1.33
1	A	693	CFZ	C4-N4	4.96	1.45	1.33
1	B	298	CFZ	C4-N4	4.96	1.45	1.33
1	A	494	CFZ	C4-N4	4.96	1.45	1.33
1	A	25	CFZ	C4-N4	4.96	1.45	1.33
1	A	96	CFZ	C4-N4	4.95	1.45	1.33
1	B	399	CFZ	C4-N4	4.95	1.45	1.33
1	A	583	CFZ	C4-N4	4.95	1.45	1.33
1	A	21	CFZ	C4-N4	4.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	CFZ	C4-N4	4.95	1.45	1.33
1	A	73	CFZ	C4-N4	4.95	1.45	1.33
1	A	161	CFZ	C4-N4	4.95	1.45	1.33
1	A	381	CFZ	C4-N4	4.95	1.45	1.33
1	B	156	CFZ	C4-N4	4.95	1.45	1.33
1	B	360	CFZ	C4-N4	4.95	1.45	1.33
1	A	382	CFZ	C4-N4	4.95	1.45	1.33
1	A	411	CFZ	C4-N4	4.95	1.45	1.33
1	B	682	CFZ	C4-N4	4.95	1.45	1.33
1	A	10	CFZ	C4-N4	4.95	1.45	1.33
1	B	353	CFZ	C4-N4	4.95	1.45	1.33
1	B	585	CFZ	C4-N4	4.95	1.45	1.33
1	B	631	CFZ	C4-N4	4.95	1.45	1.33
1	A	679	CFZ	C4-N4	4.95	1.45	1.33
1	B	232	CFZ	C4-N4	4.95	1.45	1.33
1	B	234	CFZ	C4-N4	4.95	1.45	1.33
1	B	171	CFZ	C4-N4	4.95	1.45	1.33
1	A	587	CFZ	C4-N4	4.95	1.45	1.33
1	A	655	CFZ	C4-N4	4.95	1.45	1.33
1	A	279	CFZ	C4-N4	4.95	1.45	1.33
1	B	693	CFZ	C4-N4	4.95	1.45	1.33
1	A	372	CFZ	C4-N4	4.95	1.45	1.33
1	A	625	CFZ	C4-N4	4.95	1.45	1.33
1	A	144	CFZ	C4-N4	4.95	1.45	1.33
1	A	188	CFZ	C4-N4	4.95	1.45	1.33
1	B	201	CFZ	C4-N4	4.95	1.45	1.33
1	A	530	UFT	C2-N1	4.95	1.46	1.38
1	A	308	CFZ	C4-N4	4.95	1.45	1.33
1	B	354	CFZ	C4-N4	4.95	1.45	1.33
1	A	536	CFZ	C4-N4	4.95	1.45	1.33
1	B	564	CFZ	C4-N4	4.95	1.45	1.33
1	A	285	CFZ	C4-N4	4.95	1.45	1.33
1	B	46	CFZ	C4-N4	4.95	1.45	1.33
1	A	129	CFZ	C4-N4	4.95	1.45	1.33
1	A	458	CFZ	C4-N4	4.95	1.45	1.33
1	B	592	CFZ	C4-N4	4.95	1.45	1.33
1	B	249	CFZ	C4-N4	4.95	1.45	1.33
1	B	528	CFZ	C4-N4	4.95	1.45	1.33
1	B	574	CFZ	C4-N4	4.95	1.45	1.33
1	B	49	CFZ	C4-N4	4.95	1.45	1.33
1	A	316	CFZ	C4-N4	4.95	1.45	1.33
1	B	625	CFZ	C4-N4	4.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	498	CFZ	C4-N4	4.95	1.45	1.33
1	B	511	CFZ	C4-N4	4.95	1.45	1.33
1	A	33	UFT	C2-N1	4.95	1.46	1.38
1	A	104	CFZ	C4-N4	4.95	1.45	1.33
1	B	124	CFZ	C4-N4	4.95	1.45	1.33
1	B	325	CFZ	C4-N4	4.95	1.45	1.33
1	B	441	CFZ	C4-N4	4.95	1.45	1.33
1	A	558	CFZ	C4-N4	4.95	1.45	1.33
1	B	610	CFZ	C4-N4	4.95	1.45	1.33
1	B	659	UFT	C2-N1	4.95	1.46	1.38
1	B	241	CFZ	C4-N4	4.95	1.45	1.33
1	A	518	CFZ	C4-N4	4.95	1.45	1.33
1	B	637	CFZ	C4-N4	4.95	1.45	1.33
1	B	144	CFZ	C4-N4	4.95	1.45	1.33
1	B	157	CFZ	C4-N4	4.95	1.45	1.33
1	B	565	CFZ	C4-N4	4.95	1.45	1.33
1	B	647	CFZ	C4-N4	4.95	1.45	1.33
1	B	75	CFZ	C4-N4	4.95	1.45	1.33
1	B	667	CFZ	C4-N4	4.95	1.45	1.33
1	B	26	CFZ	C4-N4	4.95	1.45	1.33
1	B	57	CFZ	C4-N4	4.95	1.45	1.33
1	A	325	CFZ	C4-N4	4.95	1.45	1.33
1	B	506	CFZ	C4-N4	4.95	1.45	1.33
1	B	184	CFZ	C4-N4	4.94	1.45	1.33
1	A	406	CFZ	C4-N4	4.94	1.45	1.33
1	A	492	CFZ	C4-N4	4.94	1.45	1.33
1	B	550	CFZ	C4-N4	4.94	1.45	1.33
1	A	585	CFZ	C4-N4	4.94	1.45	1.33
1	A	659	UFT	C2-N1	4.94	1.46	1.38
1	A	156	CFZ	C4-N4	4.94	1.45	1.33
1	B	206	CFZ	C4-N4	4.94	1.45	1.33
1	B	362	CFZ	C4-N4	4.94	1.45	1.33
1	A	399	CFZ	C4-N4	4.94	1.45	1.33
1	B	469	CFZ	C4-N4	4.94	1.45	1.33
1	A	540	CFZ	C4-N4	4.94	1.45	1.33
1	B	21	CFZ	C4-N4	4.94	1.45	1.33
1	B	67	CFZ	C4-N4	4.94	1.45	1.33
1	A	332	CFZ	C4-N4	4.94	1.45	1.33
1	B	438	CFZ	C4-N4	4.94	1.45	1.33
1	A	46	CFZ	C4-N4	4.94	1.45	1.33
1	A	242	CFZ	C4-N4	4.94	1.45	1.33
1	B	477	CFZ	C4-N4	4.94	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	576	CFZ	C4-N4	4.94	1.45	1.33
1	B	131	CFZ	C4-N4	4.94	1.45	1.33
1	A	173	CFZ	C4-N4	4.94	1.45	1.33
1	B	551	CFZ	C4-N4	4.94	1.45	1.33
1	A	418	CFZ	C4-N4	4.94	1.45	1.33
1	B	418	CFZ	C4-N4	4.94	1.45	1.33
1	A	700	CFZ	C4-N4	4.94	1.45	1.33
1	A	57	CFZ	C4-N4	4.94	1.45	1.33
1	B	246	CFZ	C4-N4	4.94	1.45	1.33
1	A	632	CFZ	C4-N4	4.94	1.45	1.33
1	B	73	CFZ	C4-N4	4.94	1.45	1.33
1	B	114	CFZ	C4-N4	4.94	1.45	1.33
1	B	406	CFZ	C4-N4	4.94	1.45	1.33
1	A	282	CFZ	C4-N4	4.94	1.45	1.33
1	B	651	CFZ	C4-N4	4.94	1.45	1.33
1	A	201	CFZ	C4-N4	4.94	1.45	1.33
1	A	378	CFZ	C4-N4	4.94	1.45	1.33
1	A	436	CFZ	C4-N4	4.94	1.45	1.33
1	B	110	CFZ	C4-N4	4.94	1.45	1.33
1	B	139	CFZ	C4-N4	4.94	1.45	1.33
1	A	384	CFZ	C4-N4	4.94	1.45	1.33
1	B	540	CFZ	C4-N4	4.94	1.45	1.33
1	A	351	CFZ	C4-N4	4.94	1.45	1.33
1	A	438	CFZ	C4-N4	4.94	1.45	1.33
1	A	218	CFZ	C4-N4	4.94	1.45	1.33
1	B	218	CFZ	C4-N4	4.94	1.45	1.33
1	B	219	CFZ	C4-N4	4.94	1.45	1.33
1	B	417	CFZ	C4-N4	4.94	1.45	1.33
1	B	308	CFZ	C4-N4	4.94	1.45	1.33
1	B	373	CFZ	C4-N4	4.94	1.45	1.33
1	B	517	CFZ	C4-N4	4.94	1.45	1.33
1	B	632	CFZ	C4-N4	4.94	1.45	1.33
1	B	698	CFZ	C4-N4	4.94	1.45	1.33
1	A	298	CFZ	C4-N4	4.94	1.45	1.33
1	A	440	CFZ	C4-N4	4.94	1.45	1.33
1	A	604	CFZ	C4-N4	4.94	1.45	1.33
1	B	604	CFZ	C4-N4	4.94	1.45	1.33
1	B	130	CFZ	C4-N4	4.94	1.45	1.33
1	B	247	CFZ	C4-N4	4.94	1.45	1.33
1	A	473	CFZ	C4-N4	4.94	1.45	1.33
1	A	246	CFZ	C4-N4	4.94	1.45	1.33
1	A	462	CFZ	C4-N4	4.94	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	CFZ	C4-N4	4.94	1.45	1.33
1	B	378	CFZ	C4-N4	4.94	1.45	1.33
1	B	643	CFZ	C4-N4	4.94	1.45	1.33
1	B	63	CFZ	C4-N4	4.94	1.45	1.33
1	A	130	CFZ	C4-N4	4.94	1.45	1.33
1	A	234	CFZ	C4-N4	4.94	1.45	1.33
1	A	198	CFZ	C4-N4	4.94	1.45	1.33
1	A	219	CFZ	C4-N4	4.94	1.45	1.33
1	B	34	CFZ	C4-N4	4.93	1.45	1.33
1	A	210	CFZ	C4-N4	4.93	1.45	1.33
1	A	603	CFZ	C4-N4	4.93	1.45	1.33
1	B	198	CFZ	C4-N4	4.93	1.45	1.33
1	A	441	CFZ	C4-N4	4.93	1.45	1.33
1	B	426	CFZ	C4-N4	4.93	1.45	1.33
1	B	603	CFZ	C4-N4	4.93	1.45	1.33
1	B	120	CFZ	C4-N4	4.93	1.45	1.33
1	B	279	CFZ	C4-N4	4.93	1.45	1.33
1	A	444	CFZ	C4-N4	4.93	1.45	1.33
1	A	550	CFZ	C4-N4	4.93	1.45	1.33
1	A	691	CFZ	C4-N4	4.93	1.45	1.33
1	B	104	CFZ	C4-N4	4.93	1.45	1.33
1	A	247	CFZ	C4-N4	4.93	1.45	1.33
1	A	455	CFZ	C4-N4	4.93	1.45	1.33
1	B	518	CFZ	C4-N4	4.93	1.45	1.33
1	B	583	CFZ	C4-N4	4.93	1.45	1.33
1	B	72	CFZ	C4-N4	4.93	1.45	1.33
1	B	151	CFZ	C4-N4	4.93	1.45	1.33
1	A	407	CFZ	C4-N4	4.93	1.45	1.33
1	B	548	CFZ	C4-N4	4.93	1.45	1.33
1	A	349	CFZ	C4-N4	4.93	1.45	1.33
1	A	387	CFZ	C4-N4	4.93	1.45	1.33
1	A	548	CFZ	C4-N4	4.93	1.45	1.33
1	A	459	CFZ	C4-N4	4.93	1.45	1.33
1	A	574	CFZ	C4-N4	4.93	1.45	1.33
1	B	704	CFZ	C4-N4	4.93	1.45	1.33
1	B	302	UFT	C2-N1	4.93	1.46	1.38
1	B	10	CFZ	C4-N4	4.93	1.45	1.33
1	B	209	CFZ	C4-N4	4.93	1.45	1.33
1	A	425	CFZ	C4-N4	4.93	1.45	1.33
1	B	459	CFZ	C4-N4	4.93	1.45	1.33
1	A	517	CFZ	C4-N4	4.93	1.45	1.33
1	A	592	CFZ	C4-N4	4.93	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	647	CFZ	C4-N4	4.93	1.45	1.33
1	B	655	CFZ	C4-N4	4.93	1.45	1.33
1	B	188	CFZ	C4-N4	4.93	1.45	1.33
1	B	458	CFZ	C4-N4	4.93	1.45	1.33
1	A	114	CFZ	C4-N4	4.93	1.45	1.33
1	B	173	CFZ	C4-N4	4.93	1.45	1.33
1	B	439	CFZ	C4-N4	4.93	1.45	1.33
1	B	338	CFZ	C4-N4	4.93	1.45	1.33
1	A	157	CFZ	C4-N4	4.93	1.45	1.33
1	B	328	CFZ	C4-N4	4.93	1.45	1.33
1	B	165	CFZ	C4-N4	4.93	1.45	1.33
1	B	323	CFZ	C4-N4	4.93	1.45	1.33
1	A	477	CFZ	C4-N4	4.93	1.45	1.33
1	B	352	UFT	C2-N1	4.93	1.46	1.38
1	B	440	CFZ	C4-N4	4.93	1.45	1.33
1	B	679	CFZ	C4-N4	4.93	1.45	1.33
1	B	103	CFZ	C4-N4	4.93	1.45	1.33
1	A	151	CFZ	C4-N4	4.93	1.45	1.33
1	B	149	CFZ	C4-N4	4.93	1.45	1.33
1	A	338	CFZ	C4-N4	4.93	1.45	1.33
1	B	39	CFZ	C4-N4	4.92	1.45	1.33
1	A	241	CFZ	C4-N4	4.92	1.45	1.33
1	A	302	UFT	C2-N1	4.92	1.46	1.38
1	B	111	CFZ	C4-N4	4.92	1.45	1.33
1	B	639	CFZ	C4-N4	4.92	1.45	1.33
1	A	439	CFZ	C4-N4	4.92	1.45	1.33
1	B	96	CFZ	C4-N4	4.92	1.45	1.33
1	A	212	CFZ	C4-N4	4.92	1.45	1.33
1	B	242	CFZ	C4-N4	4.92	1.45	1.33
1	A	362	CFZ	C4-N4	4.92	1.45	1.33
1	B	370	CFZ	C4-N4	4.92	1.45	1.33
1	A	451	CFZ	C4-N4	4.92	1.45	1.33
1	B	600	CFZ	C4-N4	4.92	1.45	1.33
1	A	614	CFZ	C4-N4	4.92	1.45	1.33
1	B	140	CFZ	C4-N4	4.92	1.45	1.33
1	A	353	CFZ	C4-N4	4.92	1.45	1.33
1	A	15	CFZ	C4-N4	4.92	1.45	1.33
1	A	120	CFZ	C4-N4	4.92	1.45	1.33
1	A	631	CFZ	C4-N4	4.92	1.45	1.33
1	A	149	CFZ	C4-N4	4.92	1.45	1.33
1	A	551	CFZ	C4-N4	4.92	1.45	1.33
1	B	512	CFZ	C4-N4	4.92	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	254	CFZ	C4-N4	4.92	1.45	1.33
1	A	506	CFZ	C4-N4	4.92	1.45	1.33
1	A	543	CFZ	C4-N4	4.92	1.45	1.33
1	A	209	CFZ	C4-N4	4.92	1.45	1.33
1	B	351	CFZ	C4-N4	4.92	1.45	1.33
1	B	372	CFZ	C4-N4	4.92	1.45	1.33
1	A	164	CFZ	C4-N4	4.92	1.45	1.33
1	B	332	CFZ	C4-N4	4.92	1.45	1.33
1	A	469	CFZ	C4-N4	4.92	1.45	1.33
1	A	26	CFZ	C4-N4	4.92	1.45	1.33
1	B	492	CFZ	C4-N4	4.92	1.45	1.33
1	B	285	CFZ	C4-N4	4.92	1.45	1.33
1	B	568	CFZ	C4-N4	4.92	1.45	1.33
1	A	232	CFZ	C4-N4	4.92	1.45	1.33
1	A	249	CFZ	C4-N4	4.92	1.45	1.33
1	A	565	CFZ	C4-N4	4.92	1.45	1.33
1	A	664	CFZ	C4-N4	4.92	1.45	1.33
1	A	682	CFZ	C4-N4	4.92	1.45	1.33
1	A	369	CFZ	C4-N4	4.92	1.45	1.33
1	B	117	CFZ	C4-N4	4.92	1.45	1.33
1	B	315	CFZ	C4-N4	4.91	1.45	1.33
1	B	15	CFZ	C4-N4	4.91	1.45	1.33
1	B	543	CFZ	C4-N4	4.91	1.45	1.33
1	A	610	CFZ	C4-N4	4.91	1.45	1.33
1	A	652	CFZ	C4-N4	4.91	1.45	1.33
1	A	704	CFZ	C4-N4	4.91	1.45	1.33
1	A	370	CFZ	C4-N4	4.91	1.45	1.33
1	B	79	CFZ	C4-N4	4.91	1.45	1.33
1	B	316	CFZ	C4-N4	4.91	1.45	1.33
1	A	90	CFZ	C4-N4	4.91	1.45	1.33
1	B	90	CFZ	C4-N4	4.91	1.45	1.33
1	A	139	CFZ	C4-N4	4.91	1.45	1.33
1	A	576	CFZ	C4-N4	4.91	1.45	1.33
1	B	196	UFT	C2-N1	4.91	1.46	1.38
1	A	404	CFZ	C4-N4	4.91	1.45	1.33
1	B	474	CFZ	C4-N4	4.91	1.45	1.33
1	A	568	CFZ	C4-N4	4.91	1.45	1.33
1	A	111	CFZ	C4-N4	4.91	1.45	1.33
1	B	28	CFZ	C4-N4	4.91	1.45	1.33
1	A	76	CFZ	C4-N4	4.91	1.45	1.33
1	A	639	CFZ	C4-N4	4.91	1.45	1.33
1	A	486	CFZ	C4-N4	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	620	CFZ	C4-N4	4.91	1.45	1.33
1	A	63	CFZ	C4-N4	4.91	1.45	1.33
1	B	536	CFZ	C4-N4	4.91	1.45	1.33
1	A	464	UFT	C2-N1	4.90	1.46	1.38
1	A	131	CFZ	C4-N4	4.90	1.45	1.33
1	B	411	CFZ	C4-N4	4.90	1.45	1.33
1	A	413	UFT	C2-N1	4.90	1.46	1.38
1	A	363	CFZ	C4-N4	4.90	1.45	1.33
1	B	556	CFZ	C4-N4	4.90	1.45	1.33
1	B	664	CFZ	C4-N4	4.90	1.45	1.33
1	A	34	CFZ	C4-N4	4.90	1.45	1.33
1	B	425	CFZ	C4-N4	4.90	1.45	1.33
1	A	124	CFZ	C4-N4	4.90	1.45	1.33
1	A	117	CFZ	C4-N4	4.90	1.45	1.33
1	B	129	CFZ	C4-N4	4.90	1.45	1.33
1	A	355	CFZ	C4-N4	4.90	1.45	1.33
1	B	405	CFZ	C4-N4	4.90	1.45	1.33
1	B	25	CFZ	C4-N4	4.90	1.45	1.33
1	A	389	UFT	C2-N1	4.90	1.46	1.38
1	A	513	UFT	C2-N1	4.89	1.46	1.38
1	A	651	CFZ	C4-N4	4.89	1.45	1.33
1	A	206	CFZ	C4-N4	4.89	1.45	1.33
1	B	387	CFZ	C4-N4	4.89	1.45	1.33
1	B	498	CFZ	C4-N4	4.89	1.45	1.33
1	B	473	CFZ	C4-N4	4.89	1.45	1.33
1	B	377	UFT	C2-N1	4.89	1.46	1.38
1	A	523	CFZ	C4-N4	4.88	1.45	1.33
1	B	335	CFZ	C4-N4	4.88	1.45	1.33
1	B	464	UFT	C2-N1	4.88	1.46	1.38
1	A	321	CFZ	C4-N4	4.88	1.45	1.33
1	A	196	UFT	C2-N1	4.87	1.46	1.38
1	A	75	CFZ	C4-N4	4.87	1.45	1.33
1	B	720	UFT	C2-N1	4.87	1.46	1.38
1	B	8	UFT	C2-N1	4.87	1.46	1.38
1	A	49	CFZ	C4-N4	4.87	1.45	1.33
1	B	321	CFZ	C4-N4	4.87	1.45	1.33
1	A	424	CFZ	C4-N4	4.87	1.45	1.33
1	A	354	CFZ	C4-N4	4.87	1.45	1.33
1	A	556	CFZ	C4-N4	4.87	1.45	1.33
1	B	494	CFZ	C4-N4	4.87	1.45	1.33
1	A	44	UFT	C2-N1	4.87	1.46	1.38
1	B	245	UFT	C2-N1	4.86	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	UFT	C2-N1	4.86	1.46	1.38
1	A	673	UFT	C2-N1	4.86	1.46	1.38
1	B	524	UFT	C2-N1	4.85	1.46	1.38
1	A	361	UFT	C2-N1	4.85	1.46	1.38
1	B	424	CFZ	C4-N4	4.85	1.45	1.33
1	A	42	UFT	C2-N1	4.85	1.46	1.38
1	B	44	UFT	C2-N1	4.84	1.46	1.38
1	B	174	UFT	C2-N1	4.84	1.46	1.38
1	B	684	UFT	C2-N1	4.83	1.46	1.38
1	A	377	UFT	C2-N1	4.83	1.46	1.38
1	B	673	UFT	C2-N1	4.83	1.46	1.38
1	A	80	UFT	C2-N1	4.83	1.46	1.38
1	B	32	UFT	C2-N1	4.83	1.46	1.38
1	A	335	CFZ	C4-N4	4.82	1.45	1.33
1	A	535	UFT	C2-N1	4.82	1.46	1.38
1	B	389	UFT	C2-N1	4.82	1.46	1.38
1	B	141	UFT	C2-N1	4.82	1.46	1.38
1	B	260	UFT	C2-N1	4.81	1.46	1.38
1	B	50	UFT	C2-N1	4.81	1.46	1.38
1	B	80	UFT	C2-N1	4.80	1.46	1.38
1	A	365	UFT	C2-N1	4.80	1.46	1.38
1	A	174	UFT	C2-N1	4.80	1.46	1.38
1	A	233	UFT	C2-N1	4.80	1.46	1.38
1	B	544	UFT	C2-N1	4.80	1.46	1.38
1	B	33	UFT	C2-N1	4.79	1.46	1.38
1	B	535	UFT	C2-N1	4.79	1.46	1.38
1	A	684	UFT	C2-N1	4.79	1.46	1.38
1	A	260	UFT	C2-N1	4.79	1.46	1.38
1	A	499	UFT	C2-N1	4.78	1.46	1.38
1	A	141	UFT	C2-N1	4.78	1.46	1.38
1	A	179	UFT	C2-N1	4.78	1.46	1.38
1	B	549	UFT	C2-N1	4.78	1.46	1.38
1	A	153	UFT	C2-N1	4.78	1.46	1.38
1	B	39	CFZ	C2'-C3'	-4.78	1.46	1.52
1	B	153	UFT	C2-N1	4.77	1.46	1.38
1	B	421	UFT	C2-N1	4.77	1.46	1.38
1	B	472	UFT	C2-N1	4.77	1.46	1.38
1	A	229	UFT	C2-N1	4.77	1.46	1.38
1	A	544	UFT	C2-N1	4.76	1.46	1.38
1	A	472	UFT	C2-N1	4.76	1.46	1.38
1	A	344	UFT	C2-N1	4.76	1.46	1.38
1	B	365	UFT	C2-N1	4.75	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	UFT	C2-N1	4.75	1.46	1.38
1	A	712	UFT	C2-N1	4.75	1.46	1.38
1	A	293	UFT	C2-N1	4.75	1.46	1.38
1	B	590	UFT	C2-N1	4.75	1.46	1.38
1	B	179	UFT	C2-N1	4.75	1.46	1.38
1	B	347	UFT	C2-N1	4.75	1.46	1.38
1	A	509	UFT	C2-N1	4.74	1.46	1.38
1	A	135	UFT	C2-N1	4.74	1.46	1.38
1	B	305	UFT	C2-N1	4.74	1.46	1.38
1	B	646	UFT	C2-N1	4.74	1.46	1.38
1	B	59	UFT	C2-N1	4.74	1.46	1.38
1	A	39	CFZ	C2'-C3'	-4.74	1.46	1.52
1	A	534	UFT	C2-N1	4.73	1.46	1.38
1	B	499	UFT	C2-N1	4.73	1.46	1.38
1	A	192	UFT	C2-N1	4.73	1.46	1.38
1	A	366	UFT	C2-N1	4.73	1.46	1.38
1	A	485	UFT	C2-N1	4.73	1.46	1.38
1	B	712	UFT	C2-N1	4.73	1.46	1.38
1	A	502	UFT	C2-N1	4.73	1.46	1.38
1	B	108	UFT	C2-N1	4.73	1.46	1.38
1	B	559	UFT	C2-N1	4.72	1.46	1.38
1	A	646	UFT	C2-N1	4.72	1.46	1.38
1	B	555	UFT	C2-N1	4.72	1.46	1.38
1	A	421	UFT	C2-N1	4.72	1.46	1.38
1	A	48	UFT	C2-N1	4.72	1.46	1.38
1	B	545	UFT	C2-N1	4.72	1.46	1.38
1	A	701	UFT	C2-N1	4.72	1.46	1.38
1	B	423	UFT	C2-N1	4.72	1.46	1.38
1	B	695	UFT	C2-N1	4.72	1.46	1.38
1	B	192	UFT	C2-N1	4.72	1.46	1.38
1	B	571	UFT	C2-N1	4.71	1.46	1.38
1	A	305	UFT	C2-N1	4.71	1.46	1.38
1	A	126	UFT	C2-N1	4.71	1.46	1.38
1	B	154	UFT	C2-N1	4.71	1.46	1.38
1	B	703	UFT	C2-N1	4.71	1.46	1.38
1	B	293	UFT	C2-N1	4.71	1.46	1.38
1	B	334	UFT	C2-N1	4.71	1.46	1.38
1	A	367	UFT	C2-N1	4.71	1.46	1.38
1	B	229	UFT	C2-N1	4.71	1.46	1.38
1	A	108	UFT	C2-N1	4.71	1.46	1.38
1	B	135	UFT	C2-N1	4.71	1.46	1.38
1	B	509	UFT	C2-N1	4.71	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	703	UFT	C2-N1	4.71	1.46	1.38
1	B	92	UFT	C2-N1	4.70	1.46	1.38
1	A	719	UFT	C2-N1	4.70	1.46	1.38
1	B	519	UFT	C2-N1	4.70	1.46	1.38
1	A	695	UFT	C2-N1	4.70	1.46	1.38
1	B	48	UFT	C2-N1	4.70	1.46	1.38
1	B	581	UFT	C2-N1	4.70	1.46	1.38
1	A	608	UFT	C2-N1	4.70	1.46	1.38
1	A	94	UFT	C2-N1	4.70	1.46	1.38
1	B	502	UFT	C2-N1	4.70	1.46	1.38
1	B	309	UFT	C2-N1	4.70	1.46	1.38
1	B	270	UFT	C2-N1	4.70	1.46	1.38
1	A	309	UFT	C2-N1	4.70	1.46	1.38
1	B	530	UFT	C2-N1	4.69	1.46	1.38
1	A	559	UFT	C2-N1	4.69	1.46	1.38
1	A	423	UFT	C2-N1	4.69	1.46	1.38
1	A	97	UFT	C2-N1	4.69	1.46	1.38
1	A	98	UFT	C2-N1	4.69	1.46	1.38
1	A	214	UFT	C2-N1	4.69	1.46	1.38
1	A	590	UFT	C2-N1	4.69	1.46	1.38
1	B	460	UFT	C2-N1	4.69	1.46	1.38
1	B	88	UFT	C2-N1	4.69	1.46	1.38
1	B	489	UFT	C2-N1	4.69	1.46	1.38
1	A	549	UFT	C2-N1	4.69	1.46	1.38
1	A	8	UFT	C2-N1	4.69	1.46	1.38
1	B	366	UFT	C2-N1	4.69	1.46	1.38
1	B	367	UFT	C2-N1	4.68	1.46	1.38
1	B	669	UFT	C2-N1	4.68	1.46	1.38
1	B	98	UFT	C2-N1	4.68	1.46	1.38
1	A	92	UFT	C2-N1	4.68	1.46	1.38
1	B	266	UFT	C2-N1	4.68	1.46	1.38
1	B	618	UFT	C2-N1	4.68	1.46	1.38
1	A	163	UFT	C2-N1	4.68	1.46	1.38
1	A	251	UFT	C2-N1	4.68	1.46	1.38
1	A	13	UFT	C2-N1	4.67	1.45	1.38
1	A	169	UFT	C2-N1	4.67	1.45	1.38
1	B	456	UFT	C2-N1	4.67	1.45	1.38
1	B	491	CFZ	C2'-C3'	-4.67	1.46	1.52
1	A	154	UFT	C2-N1	4.67	1.45	1.38
1	B	208	UFT	C2-N1	4.67	1.45	1.38
1	A	217	UFT	C2-N1	4.67	1.45	1.38
1	A	545	UFT	C2-N1	4.67	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	666	UFT	C2-N1	4.67	1.45	1.38
1	B	696	UFT	C2-N1	4.67	1.45	1.38
1	B	554	UFT	C2-N1	4.67	1.45	1.38
1	B	21	CFZ	C2'-C3'	-4.67	1.46	1.52
1	B	175	UFT	C2-N1	4.67	1.45	1.38
1	B	204	UFT	C2-N1	4.67	1.45	1.38
1	A	329	UFT	C2-N1	4.67	1.45	1.38
1	B	504	UFT	C2-N1	4.67	1.45	1.38
1	B	636	UFT	C2-N1	4.67	1.45	1.38
1	A	88	UFT	C2-N1	4.67	1.45	1.38
1	B	322	UFT	C2-N1	4.67	1.45	1.38
1	B	534	UFT	C2-N1	4.67	1.45	1.38
1	A	690	UFT	C2-N1	4.67	1.45	1.38
1	B	621	UFT	C2-N1	4.67	1.45	1.38
1	B	202	UFT	C2-N1	4.67	1.45	1.38
1	A	245	UFT	C2-N1	4.67	1.45	1.38
1	B	344	UFT	C2-N1	4.67	1.45	1.38
1	A	86	UFT	C2-N1	4.66	1.45	1.38
1	A	689	UFT	C2-N1	4.66	1.45	1.38
1	B	542	UFT	C2-N1	4.66	1.45	1.38
1	B	106	UFT	C2-N1	4.66	1.45	1.38
1	A	202	UFT	C2-N1	4.66	1.45	1.38
1	A	270	UFT	C2-N1	4.66	1.45	1.38
1	A	581	UFT	C2-N1	4.66	1.45	1.38
1	A	431	UFT	C2-N1	4.66	1.45	1.38
1	B	629	UFT	C2-N1	4.66	1.45	1.38
1	A	137	UFT	C2-N1	4.66	1.45	1.38
1	B	163	UFT	C2-N1	4.66	1.45	1.38
1	A	313	UFT	C2-N1	4.66	1.45	1.38
1	A	208	UFT	C2-N1	4.66	1.45	1.38
1	A	347	UFT	C2-N1	4.66	1.45	1.38
1	A	635	UFT	C2-N1	4.66	1.45	1.38
1	B	84	UFT	C2-N1	4.66	1.45	1.38
1	A	554	UFT	C2-N1	4.66	1.45	1.38
1	A	59	UFT	C2-N1	4.66	1.45	1.38
1	B	336	UFT	C2-N1	4.66	1.45	1.38
1	A	460	UFT	C2-N1	4.66	1.45	1.38
1	B	582	UFT	C2-N1	4.66	1.45	1.38
1	B	687	UFT	C2-N1	4.66	1.45	1.38
1	A	582	UFT	C2-N1	4.66	1.45	1.38
1	A	618	UFT	C2-N1	4.66	1.45	1.38
1	B	265	UFT	C2-N1	4.66	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	456	UFT	C2-N1	4.66	1.45	1.38
1	A	571	UFT	C2-N1	4.66	1.45	1.38
1	A	204	UFT	C2-N1	4.65	1.45	1.38
1	A	55	UFT	C2-N1	4.65	1.45	1.38
1	A	106	UFT	C2-N1	4.65	1.45	1.38
1	A	629	UFT	C2-N1	4.65	1.45	1.38
1	A	160	UFT	C2-N1	4.65	1.45	1.38
1	B	719	UFT	C2-N1	4.65	1.45	1.38
1	B	169	UFT	C2-N1	4.65	1.45	1.38
1	B	329	UFT	C2-N1	4.65	1.45	1.38
1	B	447	UFT	C2-N1	4.65	1.45	1.38
1	A	687	UFT	C2-N1	4.65	1.45	1.38
1	A	434	UFT	C2-N1	4.65	1.45	1.38
1	B	607	UFT	C2-N1	4.65	1.45	1.38
1	B	663	UFT	C2-N1	4.65	1.45	1.38
1	A	334	UFT	C2-N1	4.65	1.45	1.38
1	A	489	UFT	C2-N1	4.65	1.45	1.38
1	A	696	UFT	C2-N1	4.65	1.45	1.38
1	B	97	UFT	C2-N1	4.65	1.45	1.38
1	B	602	UFT	C2-N1	4.65	1.45	1.38
1	A	424	CFZ	C2'-C3'	-4.65	1.46	1.52
1	B	126	UFT	C2-N1	4.65	1.45	1.38
1	A	182	UFT	C2-N1	4.65	1.45	1.38
1	A	62	UFT	C2-N1	4.65	1.45	1.38
1	A	266	UFT	C2-N1	4.65	1.45	1.38
1	B	466	UFT	C2-N1	4.65	1.45	1.38
1	A	69	UFT	C2-N1	4.65	1.45	1.38
1	B	61	UFT	C2-N1	4.65	1.45	1.38
1	B	666	UFT	C2-N1	4.64	1.45	1.38
1	B	89	UFT	C2-N1	4.64	1.45	1.38
1	A	350	UFT	C2-N1	4.64	1.45	1.38
1	A	653	UFT	C2-N1	4.64	1.45	1.38
1	A	32	UFT	C2-N1	4.64	1.45	1.38
1	A	116	UFT	C2-N1	4.64	1.45	1.38
1	A	542	UFT	C2-N1	4.64	1.45	1.38
1	B	359	UFT	C2-N1	4.64	1.45	1.38
1	B	609	UFT	C2-N1	4.64	1.45	1.38
1	B	296	UFT	C2-N1	4.64	1.45	1.38
1	A	143	UFT	C2-N1	4.64	1.45	1.38
1	A	606	UFT	C2-N1	4.64	1.45	1.38
1	B	628	UFT	C2-N1	4.64	1.45	1.38
1	A	628	UFT	C2-N1	4.64	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	UFT	C2-N1	4.63	1.45	1.38
1	B	112	UFT	C2-N1	4.63	1.45	1.38
1	B	182	UFT	C2-N1	4.63	1.45	1.38
1	B	403	UFT	C2-N1	4.63	1.45	1.38
1	A	352	UFT	C2-N1	4.63	1.45	1.38
1	A	504	UFT	C2-N1	4.63	1.45	1.38
1	B	701	UFT	C2-N1	4.63	1.45	1.38
1	B	402	UFT	C2-N1	4.63	1.45	1.38
1	A	466	UFT	C2-N1	4.63	1.45	1.38
1	A	481	UFT	C2-N1	4.63	1.45	1.38
1	B	14	UFT	C6-N1	4.63	1.49	1.38
1	A	447	UFT	C2-N1	4.63	1.45	1.38
1	B	577	UFT	C2-N1	4.63	1.45	1.38
1	B	55	UFT	C2-N1	4.63	1.45	1.38
1	A	175	UFT	C2-N1	4.63	1.45	1.38
1	A	301	UFT	C2-N1	4.63	1.45	1.38
1	A	602	UFT	C2-N1	4.63	1.45	1.38
1	B	116	UFT	C2-N1	4.63	1.45	1.38
1	A	621	UFT	C2-N1	4.63	1.45	1.38
1	B	659	UFT	C6-N1	4.63	1.49	1.38
1	A	61	UFT	C2-N1	4.63	1.45	1.38
1	B	143	UFT	C2-N1	4.63	1.45	1.38
1	B	434	UFT	C2-N1	4.63	1.45	1.38
1	B	170	UFT	C2-N1	4.63	1.45	1.38
1	A	265	UFT	C2-N1	4.63	1.45	1.38
1	A	215	UFT	C2-N1	4.63	1.45	1.38
1	A	493	UFT	C2-N1	4.63	1.45	1.38
1	A	609	UFT	C2-N1	4.63	1.45	1.38
1	A	659	UFT	C6-N1	4.63	1.49	1.38
1	B	215	UFT	C2-N1	4.63	1.45	1.38
1	B	142	UFT	C2-N1	4.63	1.45	1.38
1	B	489	UFT	C6-N1	4.63	1.49	1.38
1	A	190	UFT	C2-N1	4.63	1.45	1.38
1	A	403	UFT	C2-N1	4.63	1.45	1.38
1	A	359	UFT	C6-N1	4.63	1.49	1.38
1	A	197	UFT	C2-N1	4.62	1.45	1.38
1	B	398	UFT	C2-N1	4.62	1.45	1.38
1	B	214	UFT	C2-N1	4.62	1.45	1.38
1	A	129	CFZ	C2'-C3'	-4.62	1.46	1.52
1	B	190	UFT	C2-N1	4.62	1.45	1.38
1	A	336	UFT	C2-N1	4.62	1.45	1.38
1	A	607	UFT	C2-N1	4.62	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	UFT	C2-N1	4.62	1.45	1.38
1	B	62	UFT	C2-N1	4.62	1.45	1.38
1	B	437	UFT	C2-N1	4.62	1.45	1.38
1	A	636	UFT	C2-N1	4.62	1.45	1.38
1	B	471	UFT	C2-N1	4.62	1.45	1.38
1	A	555	UFT	C2-N1	4.62	1.45	1.38
1	B	676	UFT	C6-N1	4.62	1.49	1.38
1	B	441	CFZ	C2'-C3'	-4.62	1.46	1.52
1	A	296	UFT	C2-N1	4.62	1.45	1.38
1	A	89	UFT	C2-N1	4.62	1.45	1.38
1	A	155	UFT	C2-N1	4.62	1.45	1.38
1	B	301	UFT	C2-N1	4.62	1.45	1.38
1	A	519	UFT	C2-N1	4.62	1.45	1.38
1	B	49	CFZ	C2'-C3'	-4.62	1.46	1.52
1	B	720	UFT	C6-N1	4.62	1.49	1.38
1	A	571	UFT	C6-N1	4.62	1.49	1.38
1	B	197	UFT	C2-N1	4.62	1.45	1.38
1	B	662	UFT	C2-N1	4.62	1.45	1.38
1	A	101	UFT	C2-N1	4.62	1.45	1.38
1	A	293	UFT	C6-N1	4.62	1.49	1.38
1	B	94	UFT	C2-N1	4.62	1.45	1.38
1	A	656	UFT	C2-N1	4.62	1.45	1.38
1	A	663	UFT	C2-N1	4.62	1.45	1.38
1	B	690	UFT	C2-N1	4.62	1.45	1.38
1	A	535	UFT	C6-N1	4.61	1.49	1.38
1	B	432	UFT	C2-N1	4.61	1.45	1.38
1	B	246	CFZ	C2'-C3'	-4.61	1.46	1.52
1	B	608	UFT	C2-N1	4.61	1.45	1.38
1	B	43	UFT	C6-N1	4.61	1.49	1.38
1	B	69	UFT	C2-N1	4.61	1.45	1.38
1	A	71	UFT	C2-N1	4.61	1.45	1.38
1	A	662	UFT	C2-N1	4.61	1.45	1.38
1	A	377	UFT	C6-N1	4.61	1.49	1.38
1	A	432	UFT	C2-N1	4.61	1.45	1.38
1	B	13	UFT	C2-N1	4.61	1.45	1.38
1	A	593	UFT	C2-N1	4.61	1.45	1.38
1	A	500	UFT	C2-N1	4.61	1.45	1.38
1	B	689	UFT	C2-N1	4.61	1.45	1.38
1	B	86	UFT	C2-N1	4.61	1.45	1.38
1	A	229	UFT	C6-N1	4.61	1.49	1.38
1	A	437	UFT	C2-N1	4.61	1.45	1.38
1	A	120	CFZ	C2'-C3'	-4.61	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	UFT	C2-N1	4.61	1.45	1.38
1	B	71	UFT	C2-N1	4.61	1.45	1.38
1	B	593	UFT	C2-N1	4.61	1.45	1.38
1	A	112	UFT	C2-N1	4.61	1.45	1.38
1	A	200	UFT	C2-N1	4.61	1.45	1.38
1	B	108	UFT	C6-N1	4.61	1.49	1.38
1	B	160	UFT	C2-N1	4.61	1.45	1.38
1	A	471	UFT	C2-N1	4.61	1.45	1.38
1	A	471	UFT	C6-N1	4.61	1.49	1.38
1	A	402	UFT	C2-N1	4.61	1.45	1.38
1	A	389	UFT	C6-N1	4.60	1.49	1.38
1	B	115	UFT	C2-N1	4.60	1.45	1.38
1	A	398	UFT	C2-N1	4.60	1.45	1.38
1	B	129	CFZ	C2'-C3'	-4.60	1.46	1.52
1	A	74	UFT	C2-N1	4.60	1.45	1.38
1	B	74	UFT	C2-N1	4.60	1.45	1.38
1	B	656	UFT	C2-N1	4.60	1.45	1.38
1	A	344	UFT	C6-N1	4.60	1.49	1.38
1	A	633	UFT	C2-N1	4.60	1.45	1.38
1	A	192	UFT	C6-N1	4.60	1.49	1.38
1	B	251	UFT	C2-N1	4.60	1.45	1.38
1	B	513	UFT	C6-N1	4.60	1.49	1.38
1	B	137	UFT	C2-N1	4.60	1.45	1.38
1	B	200	UFT	C2-N1	4.60	1.45	1.38
1	B	471	UFT	C6-N1	4.60	1.49	1.38
1	A	175	UFT	C6-N1	4.60	1.49	1.38
1	B	481	UFT	C2-N1	4.60	1.45	1.38
1	A	676	UFT	C6-N1	4.60	1.49	1.38
1	B	430	UFT	C2-N1	4.59	1.45	1.38
1	A	455	CFZ	C2'-C3'	-4.59	1.46	1.52
1	B	635	UFT	C2-N1	4.59	1.45	1.38
1	A	413	UFT	C6-N1	4.59	1.49	1.38
1	B	155	UFT	C2-N1	4.59	1.45	1.38
1	A	720	UFT	C2-N1	4.59	1.45	1.38
1	B	106	UFT	C6-N1	4.59	1.49	1.38
1	B	361	UFT	C2-N1	4.59	1.45	1.38
1	B	424	CFZ	C2'-C3'	-4.59	1.46	1.52
1	B	481	UFT	C6-N1	4.59	1.49	1.38
1	B	358	UFT	C6-N1	4.59	1.49	1.38
1	B	60	UFT	C2-N1	4.59	1.45	1.38
1	A	101	UFT	C6-N1	4.59	1.49	1.38
1	A	524	UFT	C6-N1	4.59	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	UFT	C2-N1	4.59	1.45	1.38
1	A	669	UFT	C2-N1	4.59	1.45	1.38
1	B	44	UFT	C6-N1	4.59	1.49	1.38
1	B	535	UFT	C6-N1	4.59	1.49	1.38
1	A	577	UFT	C2-N1	4.59	1.45	1.38
1	B	377	UFT	C6-N1	4.59	1.49	1.38
1	A	19	UFT	C6-N1	4.59	1.49	1.38
1	A	170	UFT	C2-N1	4.59	1.45	1.38
1	B	101	UFT	C6-N1	4.59	1.49	1.38
1	B	19	UFT	C2-N1	4.59	1.45	1.38
1	A	430	UFT	C2-N1	4.59	1.45	1.38
1	A	358	UFT	C6-N1	4.59	1.49	1.38
1	B	466	UFT	C6-N1	4.59	1.49	1.38
1	A	503	UFT	C2-N1	4.59	1.45	1.38
1	B	653	UFT	C2-N1	4.59	1.45	1.38
1	A	719	UFT	C6-N1	4.58	1.49	1.38
1	A	10	CFZ	C2'-C3'	-4.58	1.46	1.52
1	A	687	UFT	C6-N1	4.58	1.49	1.38
1	B	703	UFT	C6-N1	4.58	1.49	1.38
1	B	402	UFT	C6-N1	4.58	1.49	1.38
1	B	344	UFT	C6-N1	4.58	1.49	1.38
1	B	217	UFT	C2-N1	4.58	1.45	1.38
1	B	105	UFT	C6-N1	4.58	1.49	1.38
1	B	86	UFT	C6-N1	4.58	1.49	1.38
1	B	313	UFT	C6-N1	4.58	1.49	1.38
1	A	84	UFT	C2-N1	4.58	1.45	1.38
1	B	464	UFT	C6-N1	4.58	1.49	1.38
1	B	669	UFT	C6-N1	4.58	1.49	1.38
1	A	336	UFT	C6-N1	4.58	1.49	1.38
1	B	293	UFT	C6-N1	4.58	1.49	1.38
1	A	367	UFT	C6-N1	4.58	1.49	1.38
1	A	481	UFT	C6-N1	4.58	1.49	1.38
1	B	216	UFT	C6-N1	4.58	1.49	1.38
1	B	687	UFT	C6-N1	4.58	1.49	1.38
1	A	456	UFT	C6-N1	4.57	1.49	1.38
1	B	456	UFT	C6-N1	4.57	1.49	1.38
1	B	14	UFT	C2-N1	4.57	1.45	1.38
1	A	270	UFT	C6-N1	4.57	1.49	1.38
1	A	334	UFT	C6-N1	4.57	1.49	1.38
1	B	509	UFT	C6-N1	4.57	1.49	1.38
1	B	555	UFT	C6-N1	4.57	1.49	1.38
1	A	92	UFT	C6-N1	4.57	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	UFT	C6-N1	4.57	1.49	1.38
1	B	571	UFT	C6-N1	4.57	1.49	1.38
1	A	633	UFT	C6-N1	4.57	1.49	1.38
1	A	266	UFT	C6-N1	4.57	1.49	1.38
1	A	365	UFT	C6-N1	4.57	1.49	1.38
1	A	499	UFT	C6-N1	4.57	1.49	1.38
1	B	431	UFT	C2-N1	4.57	1.45	1.38
1	B	192	UFT	C6-N1	4.57	1.49	1.38
1	A	464	UFT	C6-N1	4.57	1.49	1.38
1	A	621	UFT	C6-N1	4.57	1.49	1.38
1	B	534	UFT	C6-N1	4.57	1.49	1.38
1	A	689	UFT	C6-N1	4.57	1.49	1.38
1	A	8	UFT	C6-N1	4.57	1.49	1.38
1	B	432	UFT	C6-N1	4.57	1.49	1.38
1	A	606	UFT	C6-N1	4.57	1.49	1.38
1	A	60	UFT	C2-N1	4.57	1.45	1.38
1	B	485	UFT	C2-N1	4.57	1.45	1.38
1	A	708	UFT	C2-N1	4.57	1.45	1.38
1	B	42	UFT	C6-N1	4.57	1.49	1.38
1	B	251	UFT	C6-N1	4.57	1.49	1.38
1	B	352	UFT	C6-N1	4.57	1.49	1.38
1	A	366	UFT	C6-N1	4.57	1.49	1.38
1	B	500	UFT	C2-N1	4.57	1.45	1.38
1	B	80	UFT	C6-N1	4.57	1.49	1.38
1	A	108	UFT	C6-N1	4.57	1.49	1.38
1	A	607	UFT	C6-N1	4.57	1.49	1.38
1	B	76	CFZ	C2'-C3'	-4.57	1.46	1.52
1	A	544	UFT	C6-N1	4.57	1.49	1.38
1	A	684	UFT	C6-N1	4.57	1.49	1.38
1	B	59	UFT	C6-N1	4.57	1.49	1.38
1	B	182	UFT	C6-N1	4.57	1.49	1.38
1	B	120	CFZ	C2'-C3'	-4.57	1.46	1.52
1	A	279	CFZ	C2'-C3'	-4.57	1.46	1.52
1	B	334	UFT	C6-N1	4.57	1.49	1.38
1	B	577	UFT	C6-N1	4.57	1.49	1.38
1	A	720	UFT	C6-N1	4.57	1.49	1.38
1	A	156	CFZ	C2'-C3'	-4.57	1.46	1.52
1	B	196	UFT	C6-N1	4.57	1.49	1.38
1	A	214	UFT	C6-N1	4.57	1.49	1.38
1	A	509	UFT	C6-N1	4.57	1.49	1.38
1	A	190	UFT	C6-N1	4.57	1.49	1.38
1	B	696	UFT	C6-N1	4.57	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	UFT	C6-N1	4.57	1.49	1.38
1	B	219	CFZ	C2'-C3'	-4.56	1.46	1.52
1	B	367	UFT	C6-N1	4.56	1.49	1.38
1	A	105	UFT	C6-N1	4.56	1.49	1.38
1	A	106	UFT	C6-N1	4.56	1.49	1.38
1	B	582	UFT	C6-N1	4.56	1.49	1.38
1	A	662	UFT	C6-N1	4.56	1.49	1.38
1	B	689	UFT	C6-N1	4.56	1.49	1.38
1	B	283	UFT	C2-N1	4.56	1.45	1.38
1	A	42	UFT	C6-N1	4.56	1.49	1.38
1	A	513	UFT	C6-N1	4.56	1.49	1.38
1	B	524	UFT	C6-N1	4.56	1.49	1.38
1	A	387	CFZ	C2'-C3'	-4.56	1.46	1.52
1	B	387	CFZ	C2'-C3'	-4.56	1.46	1.52
1	B	50	UFT	C6-N1	4.56	1.49	1.38
1	B	142	UFT	C6-N1	4.56	1.49	1.38
1	B	701	UFT	C6-N1	4.56	1.49	1.38
1	A	11	UFT	C2-N1	4.56	1.45	1.38
1	A	581	UFT	C6-N1	4.56	1.49	1.38
1	B	485	UFT	C6-N1	4.56	1.49	1.38
1	A	251	UFT	C6-N1	4.56	1.49	1.38
1	A	283	UFT	C2-N1	4.56	1.45	1.38
1	A	431	UFT	C6-N1	4.56	1.49	1.38
1	B	635	UFT	C6-N1	4.56	1.49	1.38
1	B	126	UFT	C6-N1	4.56	1.49	1.38
1	A	329	UFT	C6-N1	4.56	1.49	1.38
1	B	437	UFT	C6-N1	4.56	1.49	1.38
1	A	196	UFT	C6-N1	4.56	1.49	1.38
1	A	466	UFT	C6-N1	4.56	1.49	1.38
1	B	502	UFT	C6-N1	4.56	1.49	1.38
1	A	32	UFT	C6-N1	4.56	1.49	1.38
1	A	502	UFT	C6-N1	4.56	1.49	1.38
1	B	690	UFT	C6-N1	4.56	1.49	1.38
1	B	633	UFT	C2-N1	4.56	1.45	1.38
1	A	50	UFT	C6-N1	4.56	1.49	1.38
1	B	94	UFT	C6-N1	4.56	1.49	1.38
1	A	545	UFT	C6-N1	4.56	1.49	1.38
1	A	137	UFT	C6-N1	4.56	1.49	1.38
1	A	542	UFT	C6-N1	4.56	1.49	1.38
1	A	55	UFT	C6-N1	4.56	1.49	1.38
1	B	84	UFT	C6-N1	4.56	1.49	1.38
1	A	534	UFT	C6-N1	4.56	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	313	UFT	C2-N1	4.56	1.45	1.38
1	B	11	UFT	C6-N1	4.56	1.49	1.38
1	B	347	UFT	C6-N1	4.56	1.49	1.38
1	A	423	UFT	C6-N1	4.56	1.49	1.38
1	A	695	UFT	C6-N1	4.56	1.49	1.38
1	A	13	UFT	C6-N1	4.56	1.49	1.38
1	A	179	UFT	C6-N1	4.56	1.49	1.38
1	B	233	UFT	C6-N1	4.56	1.49	1.38
1	A	361	UFT	C6-N1	4.56	1.49	1.38
1	A	609	UFT	C6-N1	4.56	1.49	1.38
1	B	629	UFT	C6-N1	4.56	1.49	1.38
1	B	355	CFZ	C2'-C3'	-4.56	1.46	1.52
1	B	545	UFT	C6-N1	4.55	1.49	1.38
1	B	447	UFT	C6-N1	4.55	1.49	1.38
1	B	695	UFT	C6-N1	4.55	1.49	1.38
1	B	163	UFT	C6-N1	4.55	1.49	1.38
1	A	126	UFT	C6-N1	4.55	1.49	1.38
1	B	229	UFT	C6-N1	4.55	1.49	1.38
1	B	245	UFT	C6-N1	4.55	1.49	1.38
1	B	266	UFT	C6-N1	4.55	1.49	1.38
1	A	460	UFT	C6-N1	4.55	1.49	1.38
1	A	577	UFT	C6-N1	4.55	1.49	1.38
1	B	153	UFT	C6-N1	4.55	1.49	1.38
1	B	301	UFT	C6-N1	4.55	1.49	1.38
1	A	309	UFT	C6-N1	4.55	1.49	1.38
1	A	350	UFT	C6-N1	4.55	1.49	1.38
1	A	504	UFT	C6-N1	4.55	1.49	1.38
1	A	593	UFT	C6-N1	4.55	1.49	1.38
1	A	629	UFT	C6-N1	4.55	1.49	1.38
1	B	609	UFT	C6-N1	4.55	1.49	1.38
1	B	336	UFT	C6-N1	4.55	1.49	1.38
1	B	499	UFT	C6-N1	4.55	1.49	1.38
1	A	703	UFT	C6-N1	4.55	1.49	1.38
1	A	141	UFT	C6-N1	4.55	1.49	1.38
1	A	233	UFT	C6-N1	4.55	1.49	1.38
1	A	21	CFZ	C2'-C3'	-4.55	1.46	1.52
1	B	115	UFT	C6-N1	4.55	1.49	1.38
1	A	208	UFT	C6-N1	4.55	1.49	1.38
1	B	141	UFT	C6-N1	4.55	1.49	1.38
1	A	519	UFT	C6-N1	4.55	1.49	1.38
1	A	673	UFT	C6-N1	4.55	1.49	1.38
1	B	684	UFT	C6-N1	4.55	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	UFT	C6-N1	4.55	1.49	1.38
1	B	559	UFT	C6-N1	4.55	1.49	1.38
1	A	701	UFT	C6-N1	4.55	1.49	1.38
1	A	43	UFT	C6-N1	4.55	1.49	1.38
1	B	155	UFT	C6-N1	4.55	1.49	1.38
1	A	421	UFT	C6-N1	4.55	1.49	1.38
1	A	708	UFT	C6-N1	4.55	1.49	1.38
1	A	104	CFZ	C2'-C3'	-4.55	1.46	1.52
1	B	98	UFT	C6-N1	4.55	1.49	1.38
1	B	460	UFT	C6-N1	4.55	1.49	1.38
1	B	549	UFT	C6-N1	4.55	1.49	1.38
1	B	434	UFT	C6-N1	4.55	1.49	1.38
1	B	673	UFT	C6-N1	4.55	1.49	1.38
1	B	708	UFT	C2-N1	4.55	1.45	1.38
1	A	143	UFT	C6-N1	4.55	1.49	1.38
1	B	175	UFT	C6-N1	4.55	1.49	1.38
1	A	260	UFT	C6-N1	4.55	1.49	1.38
1	A	485	UFT	C6-N1	4.55	1.49	1.38
1	A	554	UFT	C6-N1	4.55	1.49	1.38
1	A	635	UFT	C6-N1	4.55	1.49	1.38
1	A	565	CFZ	C2'-C3'	-4.55	1.46	1.52
1	B	19	UFT	C6-N1	4.55	1.49	1.38
1	B	160	UFT	C6-N1	4.55	1.49	1.38
1	A	530	UFT	C6-N1	4.55	1.49	1.38
1	B	633	UFT	C6-N1	4.55	1.49	1.38
1	B	606	UFT	C2-N1	4.55	1.45	1.38
1	B	33	UFT	C6-N1	4.55	1.49	1.38
1	B	55	UFT	C6-N1	4.55	1.49	1.38
1	A	80	UFT	C6-N1	4.55	1.49	1.38
1	B	137	UFT	C6-N1	4.55	1.49	1.38
1	A	302	UFT	C6-N1	4.55	1.49	1.38
1	B	359	UFT	C6-N1	4.55	1.49	1.38
1	B	389	UFT	C6-N1	4.55	1.49	1.38
1	B	602	UFT	C6-N1	4.55	1.49	1.38
1	A	447	UFT	C6-N1	4.55	1.49	1.38
1	A	590	UFT	C6-N1	4.55	1.49	1.38
1	B	92	UFT	C6-N1	4.55	1.49	1.38
1	B	116	UFT	C6-N1	4.55	1.49	1.38
1	B	653	UFT	C6-N1	4.55	1.49	1.38
1	B	61	UFT	C6-N1	4.54	1.49	1.38
1	A	154	UFT	C6-N1	4.54	1.49	1.38
1	A	182	UFT	C6-N1	4.54	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	UFT	C6-N1	4.54	1.49	1.38
1	A	265	UFT	C6-N1	4.54	1.49	1.38
1	B	265	UFT	C6-N1	4.54	1.49	1.38
1	A	582	UFT	C6-N1	4.54	1.49	1.38
1	A	458	CFZ	C2'-C3'	-4.54	1.46	1.52
1	A	94	UFT	C6-N1	4.54	1.49	1.38
1	B	283	UFT	C6-N1	4.54	1.49	1.38
1	A	653	UFT	C6-N1	4.54	1.49	1.38
1	B	708	UFT	C6-N1	4.54	1.49	1.38
1	A	398	UFT	C6-N1	4.54	1.49	1.38
1	A	142	UFT	C6-N1	4.54	1.49	1.38
1	B	554	UFT	C6-N1	4.54	1.49	1.38
1	A	402	UFT	C6-N1	4.54	1.49	1.38
1	B	712	UFT	C6-N1	4.54	1.49	1.38
1	A	425	CFZ	C2'-C3'	-4.54	1.46	1.52
1	A	11	UFT	C6-N1	4.54	1.49	1.38
1	B	202	UFT	C6-N1	4.54	1.49	1.38
1	A	169	UFT	C6-N1	4.54	1.49	1.38
1	A	322	UFT	C6-N1	4.54	1.49	1.38
1	A	403	UFT	C6-N1	4.54	1.49	1.38
1	A	500	UFT	C6-N1	4.54	1.49	1.38
1	B	197	UFT	C6-N1	4.54	1.49	1.38
1	A	84	UFT	C6-N1	4.54	1.49	1.38
1	A	153	UFT	C6-N1	4.54	1.49	1.38
1	B	305	UFT	C6-N1	4.54	1.49	1.38
1	A	434	UFT	C6-N1	4.54	1.49	1.38
1	A	696	UFT	C6-N1	4.54	1.49	1.38
1	A	305	UFT	C6-N1	4.54	1.49	1.38
1	A	489	UFT	C6-N1	4.54	1.49	1.38
1	B	593	UFT	C6-N1	4.54	1.49	1.38
1	A	636	UFT	C6-N1	4.54	1.49	1.38
1	A	690	UFT	C6-N1	4.54	1.49	1.38
1	A	86	UFT	C6-N1	4.54	1.49	1.38
1	A	296	UFT	C6-N1	4.54	1.49	1.38
1	A	115	UFT	C6-N1	4.54	1.49	1.38
1	B	590	UFT	C6-N1	4.54	1.49	1.38
1	A	712	UFT	C6-N1	4.54	1.49	1.38
1	B	260	UFT	C6-N1	4.54	1.49	1.38
1	A	618	UFT	C6-N1	4.54	1.49	1.38
1	B	472	UFT	C6-N1	4.54	1.49	1.38
1	B	88	UFT	C6-N1	4.54	1.48	1.38
1	A	669	UFT	C6-N1	4.54	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	365	UFT	C6-N1	4.54	1.48	1.38
1	B	600	CFZ	C2'-C3'	-4.54	1.46	1.52
1	A	301	UFT	C6-N1	4.54	1.48	1.38
1	A	165	CFZ	C2'-C3'	-4.54	1.46	1.52
1	B	48	UFT	C6-N1	4.54	1.48	1.38
1	B	214	UFT	C6-N1	4.54	1.48	1.38
1	B	544	UFT	C6-N1	4.54	1.48	1.38
1	A	74	UFT	C6-N1	4.54	1.48	1.38
1	B	143	UFT	C6-N1	4.54	1.48	1.38
1	A	163	UFT	C6-N1	4.54	1.48	1.38
1	B	69	UFT	C6-N1	4.54	1.48	1.38
1	A	283	UFT	C6-N1	4.54	1.48	1.38
1	B	504	UFT	C6-N1	4.54	1.48	1.38
1	B	309	UFT	C6-N1	4.53	1.48	1.38
1	B	13	UFT	C6-N1	4.53	1.48	1.38
1	A	202	UFT	C6-N1	4.53	1.48	1.38
1	B	423	UFT	C6-N1	4.53	1.48	1.38
1	A	472	UFT	C6-N1	4.53	1.48	1.38
1	B	618	UFT	C6-N1	4.53	1.48	1.38
1	B	62	UFT	C6-N1	4.53	1.48	1.38
1	A	116	UFT	C6-N1	4.53	1.48	1.38
1	B	174	UFT	C6-N1	4.53	1.48	1.38
1	B	156	CFZ	C2'-C3'	-4.53	1.46	1.52
1	A	430	UFT	C6-N1	4.53	1.48	1.38
1	B	666	UFT	C6-N1	4.53	1.48	1.38
1	A	88	UFT	C6-N1	4.53	1.48	1.38
1	A	555	UFT	C6-N1	4.53	1.48	1.38
1	B	179	UFT	C6-N1	4.53	1.48	1.38
1	B	322	UFT	C6-N1	4.53	1.48	1.38
1	A	666	UFT	C6-N1	4.53	1.48	1.38
1	A	441	CFZ	C2'-C3'	-4.53	1.46	1.52
1	B	581	UFT	C6-N1	4.53	1.48	1.38
1	A	61	UFT	C6-N1	4.53	1.48	1.38
1	B	421	UFT	C6-N1	4.53	1.48	1.38
1	A	48	UFT	C6-N1	4.53	1.48	1.38
1	B	542	UFT	C6-N1	4.53	1.48	1.38
1	B	170	UFT	C6-N1	4.53	1.48	1.38
1	B	208	UFT	C6-N1	4.53	1.48	1.38
1	B	398	UFT	C6-N1	4.53	1.48	1.38
1	A	97	UFT	C6-N1	4.53	1.48	1.38
1	B	329	UFT	C6-N1	4.53	1.48	1.38
1	B	89	UFT	C6-N1	4.53	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	493	UFT	C6-N1	4.53	1.48	1.38
1	B	500	UFT	C6-N1	4.53	1.48	1.38
1	B	530	UFT	C6-N1	4.53	1.48	1.38
1	B	565	CFZ	C2'-C3'	-4.53	1.46	1.52
1	A	44	UFT	C6-N1	4.53	1.48	1.38
1	A	313	UFT	C6-N1	4.53	1.48	1.38
1	B	607	UFT	C6-N1	4.53	1.48	1.38
1	B	46	CFZ	C2'-C3'	-4.53	1.46	1.52
1	B	662	UFT	C6-N1	4.53	1.48	1.38
1	B	606	UFT	C6-N1	4.53	1.48	1.38
1	A	89	UFT	C6-N1	4.53	1.48	1.38
1	B	215	UFT	C6-N1	4.53	1.48	1.38
1	B	494	CFZ	C2'-C3'	-4.53	1.46	1.52
1	B	97	UFT	C6-N1	4.52	1.48	1.38
1	A	69	UFT	C6-N1	4.52	1.48	1.38
1	A	246	CFZ	C2'-C3'	-4.52	1.46	1.52
1	B	302	UFT	C6-N1	4.52	1.48	1.38
1	A	245	UFT	C6-N1	4.52	1.48	1.38
1	B	493	UFT	C6-N1	4.52	1.48	1.38
1	B	366	UFT	C6-N1	4.52	1.48	1.38
1	A	663	UFT	C6-N1	4.52	1.48	1.38
1	B	628	UFT	C6-N1	4.52	1.48	1.38
1	B	719	UFT	C6-N1	4.52	1.48	1.38
1	A	551	CFZ	C2'-C3'	-4.52	1.46	1.52
1	B	682	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	59	UFT	C6-N1	4.52	1.48	1.38
1	A	347	UFT	C6-N1	4.52	1.48	1.38
1	B	104	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	219	CFZ	C2'-C3'	-4.52	1.46	1.52
1	B	204	UFT	C6-N1	4.52	1.48	1.38
1	A	200	UFT	C6-N1	4.52	1.48	1.38
1	B	403	UFT	C6-N1	4.52	1.48	1.38
1	B	431	UFT	C6-N1	4.52	1.48	1.38
1	B	621	UFT	C6-N1	4.52	1.48	1.38
1	A	160	UFT	C6-N1	4.52	1.48	1.38
1	B	270	UFT	C6-N1	4.52	1.48	1.38
1	B	296	UFT	C6-N1	4.52	1.48	1.38
1	B	209	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	135	UFT	C6-N1	4.52	1.48	1.38
1	A	174	UFT	C6-N1	4.52	1.48	1.38
1	A	155	UFT	C6-N1	4.52	1.48	1.38
1	A	124	CFZ	C2'-C3'	-4.52	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	UFT	C6-N1	4.52	1.48	1.38
1	A	60	UFT	C6-N1	4.52	1.48	1.38
1	B	636	UFT	C6-N1	4.52	1.48	1.38
1	B	247	CFZ	C2'-C3'	-4.52	1.46	1.52
1	B	157	CFZ	C2'-C3'	-4.52	1.46	1.52
1	B	519	UFT	C6-N1	4.51	1.48	1.38
1	B	430	UFT	C6-N1	4.51	1.48	1.38
1	B	169	UFT	C6-N1	4.51	1.48	1.38
1	B	217	UFT	C6-N1	4.51	1.48	1.38
1	B	550	CFZ	C2'-C3'	-4.51	1.46	1.52
1	B	608	UFT	C6-N1	4.51	1.48	1.38
1	B	458	CFZ	C2'-C3'	-4.51	1.46	1.52
1	A	503	UFT	C6-N1	4.51	1.48	1.38
1	B	663	UFT	C6-N1	4.51	1.48	1.38
1	B	74	UFT	C6-N1	4.51	1.48	1.38
1	A	646	UFT	C6-N1	4.51	1.48	1.38
1	A	602	UFT	C6-N1	4.51	1.48	1.38
1	A	608	UFT	C6-N1	4.51	1.48	1.38
1	B	298	CFZ	C2'-C3'	-4.51	1.46	1.52
1	A	204	UFT	C6-N1	4.51	1.48	1.38
1	A	19	UFT	C2-N1	4.51	1.45	1.38
1	B	60	UFT	C6-N1	4.51	1.48	1.38
1	A	112	UFT	C6-N1	4.51	1.48	1.38
1	A	33	UFT	C6-N1	4.51	1.48	1.38
1	A	540	CFZ	C2'-C3'	-4.51	1.46	1.52
1	A	549	UFT	C6-N1	4.51	1.48	1.38
1	B	425	CFZ	C2'-C3'	-4.51	1.46	1.52
1	A	197	UFT	C6-N1	4.50	1.48	1.38
1	B	112	UFT	C6-N1	4.50	1.48	1.38
1	B	135	UFT	C6-N1	4.50	1.48	1.38
1	B	8	UFT	C6-N1	4.50	1.48	1.38
1	B	477	CFZ	C2'-C3'	-4.50	1.46	1.52
1	A	559	UFT	C6-N1	4.50	1.48	1.38
1	B	646	UFT	C6-N1	4.50	1.48	1.38
1	A	437	UFT	C6-N1	4.50	1.48	1.38
1	A	568	CFZ	C2'-C3'	-4.50	1.46	1.52
1	A	71	UFT	C6-N1	4.50	1.48	1.38
1	A	432	UFT	C6-N1	4.50	1.48	1.38
1	B	154	UFT	C6-N1	4.50	1.48	1.38
1	A	46	CFZ	C2'-C3'	-4.50	1.46	1.52
1	A	62	UFT	C6-N1	4.50	1.48	1.38
1	B	165	CFZ	C2'-C3'	-4.50	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	CFZ	C2'-C3'	-4.50	1.46	1.52
1	B	568	CFZ	C2'-C3'	-4.50	1.46	1.52
1	A	528	CFZ	C2'-C3'	-4.49	1.46	1.52
1	B	184	CFZ	C2'-C3'	-4.49	1.46	1.52
1	A	436	CFZ	C2'-C3'	-4.49	1.46	1.52
1	A	98	UFT	C6-N1	4.49	1.48	1.38
1	A	352	UFT	C6-N1	4.49	1.48	1.38
1	A	298	CFZ	C2'-C3'	-4.49	1.46	1.52
1	A	217	UFT	C6-N1	4.49	1.48	1.38
1	A	325	CFZ	C2'-C3'	-4.48	1.46	1.52
1	A	656	UFT	C6-N1	4.48	1.48	1.38
1	B	693	CFZ	C2'-C3'	-4.48	1.46	1.52
1	B	698	CFZ	C2'-C3'	-4.48	1.46	1.52
1	B	361	UFT	C6-N1	4.48	1.48	1.38
1	B	551	CFZ	C2'-C3'	-4.48	1.46	1.52
1	A	587	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	477	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	209	CFZ	C2'-C3'	-4.47	1.46	1.52
1	B	316	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	406	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	628	UFT	C6-N1	4.47	1.48	1.38
1	A	188	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	323	CFZ	C2'-C3'	-4.47	1.46	1.52
1	B	511	CFZ	C2'-C3'	-4.47	1.46	1.52
1	B	323	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	316	CFZ	C2'-C3'	-4.47	1.46	1.52
1	B	700	CFZ	C2'-C3'	-4.46	1.46	1.52
1	A	698	CFZ	C2'-C3'	-4.46	1.46	1.52
1	B	381	CFZ	C2'-C3'	-4.46	1.46	1.52
1	B	279	CFZ	C2'-C3'	-4.46	1.46	1.52
1	A	439	CFZ	C2'-C3'	-4.46	1.46	1.52
1	B	411	CFZ	C2'-C3'	-4.46	1.46	1.52
1	A	652	CFZ	C2'-C3'	-4.46	1.46	1.52
1	A	511	CFZ	C2'-C3'	-4.46	1.46	1.52
1	B	351	CFZ	C2'-C3'	-4.46	1.46	1.52
1	B	587	CFZ	C2'-C3'	-4.46	1.46	1.52
1	A	49	CFZ	C2'-C3'	-4.46	1.46	1.52
1	B	285	CFZ	C2'-C3'	-4.45	1.46	1.52
1	A	600	CFZ	C2'-C3'	-4.45	1.46	1.52
1	A	157	CFZ	C2'-C3'	-4.45	1.46	1.52
1	B	643	CFZ	C2'-C3'	-4.45	1.46	1.52
1	A	130	CFZ	C2'-C3'	-4.45	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	540	CFZ	C2'-C3'	-4.45	1.46	1.52
1	B	32	UFT	C6-N1	4.45	1.48	1.38
1	A	34	CFZ	C2'-C3'	-4.45	1.46	1.52
1	A	285	CFZ	C2'-C3'	-4.45	1.46	1.52
1	A	372	CFZ	C2'-C3'	-4.45	1.46	1.52
1	B	124	CFZ	C2'-C3'	-4.44	1.46	1.52
1	B	585	CFZ	C2'-C3'	-4.44	1.46	1.52
1	B	28	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	643	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	585	CFZ	C2'-C3'	-4.44	1.46	1.52
1	B	188	CFZ	C2'-C3'	-4.44	1.46	1.52
1	B	332	CFZ	C2'-C3'	-4.44	1.46	1.52
1	B	656	UFT	C6-N1	4.44	1.48	1.38
1	B	110	CFZ	C2'-C3'	-4.44	1.46	1.52
1	B	73	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	164	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	247	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	381	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	304	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	249	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	369	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	682	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	67	CFZ	C2'-C3'	-4.43	1.46	1.52
1	B	249	CFZ	C2'-C3'	-4.43	1.46	1.52
1	B	151	CFZ	C2'-C3'	-4.43	1.46	1.52
1	B	651	CFZ	C2'-C3'	-4.43	1.46	1.52
1	A	523	CFZ	C2'-C3'	-4.43	1.46	1.52
1	A	363	CFZ	C2'-C3'	-4.43	1.46	1.52
1	B	304	CFZ	C2'-C3'	-4.43	1.46	1.52
1	A	349	CFZ	C2'-C3'	-4.43	1.46	1.52
1	A	693	CFZ	C2'-C3'	-4.43	1.46	1.52
1	A	338	CFZ	C2'-C3'	-4.43	1.46	1.52
1	B	704	CFZ	C2'-C3'	-4.43	1.46	1.52
1	A	370	CFZ	C2'-C3'	-4.42	1.46	1.52
1	B	335	CFZ	C2'-C3'	-4.42	1.46	1.52
1	B	370	CFZ	C2'-C3'	-4.42	1.46	1.52
1	A	462	CFZ	C2'-C3'	-4.42	1.46	1.52
1	B	363	CFZ	C2'-C3'	-4.42	1.46	1.52
1	B	603	CFZ	C2'-C3'	-4.42	1.46	1.52
1	B	57	CFZ	C2'-C3'	-4.42	1.46	1.52
1	A	110	CFZ	C2'-C3'	-4.42	1.46	1.52
1	A	704	CFZ	C2'-C3'	-4.42	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	411	CFZ	C2'-C3'	-4.42	1.46	1.52
1	B	512	CFZ	C2'-C3'	-4.42	1.46	1.52
1	A	651	CFZ	C2'-C3'	-4.42	1.46	1.52
1	A	151	CFZ	C2'-C3'	-4.41	1.46	1.52
1	B	579	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	655	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	647	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	79	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	242	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	579	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	399	CFZ	C2'-C3'	-4.41	1.46	1.52
1	B	528	CFZ	C2'-C3'	-4.41	1.46	1.52
1	B	164	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	426	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	73	CFZ	C2'-C3'	-4.41	1.46	1.52
1	B	492	CFZ	C2'-C3'	-4.41	1.46	1.52
1	B	130	CFZ	C2'-C3'	-4.40	1.46	1.52
1	A	603	CFZ	C2'-C3'	-4.40	1.46	1.52
1	B	406	CFZ	C2'-C3'	-4.40	1.46	1.52
1	B	548	CFZ	C2'-C3'	-4.40	1.46	1.52
1	B	372	CFZ	C2'-C3'	-4.40	1.46	1.52
1	A	335	CFZ	C2'-C3'	-4.40	1.46	1.52
1	B	647	CFZ	C2'-C3'	-4.40	1.46	1.52
1	B	614	CFZ	C2'-C3'	-4.40	1.46	1.52
1	B	652	CFZ	C2'-C3'	-4.40	1.46	1.52
1	B	206	CFZ	C2'-C3'	-4.39	1.46	1.52
1	A	558	CFZ	C2'-C3'	-4.39	1.46	1.52
1	A	614	CFZ	C2'-C3'	-4.39	1.46	1.52
1	B	149	CFZ	C2'-C3'	-4.39	1.46	1.52
1	A	667	CFZ	C2'-C3'	-4.39	1.46	1.52
1	B	506	CFZ	C2'-C3'	-4.39	1.46	1.52
1	B	369	CFZ	C2'-C3'	-4.39	1.46	1.52
1	B	639	CFZ	C2'-C3'	-4.39	1.46	1.52
1	A	407	CFZ	C2'-C3'	-4.39	1.46	1.52
1	B	574	CFZ	C2'-C3'	-4.39	1.46	1.52
1	A	14	UFT	C2-N1	4.38	1.45	1.38
1	B	75	CFZ	C2'-C3'	-4.38	1.46	1.52
1	A	215	UFT	C6-N1	4.38	1.48	1.38
1	A	332	CFZ	C2'-C3'	-4.38	1.46	1.52
1	A	491	CFZ	C2'-C3'	-4.38	1.46	1.52
1	B	426	CFZ	C2'-C3'	-4.38	1.46	1.52
1	A	550	CFZ	C2'-C3'	-4.38	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	CFZ	C2'-C3'	-4.38	1.46	1.52
1	A	474	CFZ	C2'-C3'	-4.38	1.46	1.52
1	A	576	CFZ	C2'-C3'	-4.38	1.46	1.52
1	A	700	CFZ	C2'-C3'	-4.38	1.46	1.52
1	A	625	CFZ	C2'-C3'	-4.38	1.46	1.52
1	A	321	CFZ	C2'-C3'	-4.38	1.46	1.52
1	B	405	CFZ	C2'-C3'	-4.38	1.46	1.52
1	B	325	CFZ	C2'-C3'	-4.38	1.46	1.52
1	B	631	CFZ	C2'-C3'	-4.37	1.46	1.52
1	B	242	CFZ	C2'-C3'	-4.37	1.46	1.52
1	A	506	CFZ	C2'-C3'	-4.37	1.46	1.52
1	A	57	CFZ	C2'-C3'	-4.37	1.46	1.52
1	A	639	CFZ	C2'-C3'	-4.37	1.46	1.52
1	A	131	CFZ	C2'-C3'	-4.37	1.46	1.52
1	B	655	CFZ	C2'-C3'	-4.37	1.46	1.52
1	A	405	CFZ	C2'-C3'	-4.37	1.46	1.52
1	B	378	CFZ	C2'-C3'	-4.37	1.46	1.52
1	A	206	CFZ	C2'-C3'	-4.37	1.46	1.52
1	A	254	CFZ	C2'-C3'	-4.36	1.46	1.52
1	A	384	CFZ	C2'-C3'	-4.36	1.46	1.52
1	B	407	CFZ	C2'-C3'	-4.36	1.46	1.52
1	B	564	CFZ	C2'-C3'	-4.36	1.46	1.52
1	B	72	CFZ	C2'-C3'	-4.36	1.46	1.52
1	A	486	CFZ	C2'-C3'	-4.36	1.46	1.52
1	B	517	CFZ	C2'-C3'	-4.36	1.46	1.52
1	A	28	CFZ	C2'-C3'	-4.36	1.46	1.52
1	A	72	CFZ	C2'-C3'	-4.36	1.46	1.52
1	B	440	CFZ	C2'-C3'	-4.36	1.46	1.52
1	B	198	CFZ	C2'-C3'	-4.35	1.46	1.52
1	B	139	CFZ	C2'-C3'	-4.35	1.46	1.52
1	B	399	CFZ	C2'-C3'	-4.35	1.46	1.52
1	A	494	CFZ	C2'-C3'	-4.35	1.46	1.52
1	B	558	CFZ	C2'-C3'	-4.35	1.46	1.52
1	A	548	CFZ	C2'-C3'	-4.35	1.46	1.52
1	B	79	CFZ	C2'-C3'	-4.35	1.46	1.52
1	A	139	CFZ	C2'-C3'	-4.35	1.46	1.52
1	A	149	CFZ	C2'-C3'	-4.35	1.46	1.52
1	A	216	UFT	C6-N1	4.35	1.48	1.38
1	B	667	CFZ	C2'-C3'	-4.35	1.46	1.52
1	B	474	CFZ	C2'-C3'	-4.34	1.46	1.52
1	B	604	CFZ	C2'-C3'	-4.34	1.46	1.52
1	A	451	CFZ	C2'-C3'	-4.34	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	543	CFZ	C2'-C3'	-4.34	1.46	1.52
1	B	354	CFZ	C2'-C3'	-4.34	1.46	1.52
1	A	198	CFZ	C2'-C3'	-4.34	1.46	1.52
1	A	604	CFZ	C2'-C3'	-4.34	1.46	1.52
1	A	679	CFZ	C2'-C3'	-4.34	1.46	1.52
1	A	76	CFZ	C2'-C3'	-4.34	1.46	1.52
1	A	315	CFZ	C2'-C3'	-4.34	1.46	1.52
1	A	564	CFZ	C2'-C3'	-4.34	1.46	1.52
1	A	512	CFZ	C2'-C3'	-4.34	1.46	1.52
1	A	536	CFZ	C2'-C3'	-4.34	1.46	1.52
1	B	201	CFZ	C2'-C3'	-4.34	1.46	1.52
1	B	373	CFZ	C2'-C3'	-4.34	1.46	1.52
1	B	111	CFZ	C2'-C3'	-4.33	1.46	1.52
1	A	524	UFT	C2'-C3'	-4.33	1.46	1.52
1	B	679	CFZ	C2'-C3'	-4.33	1.46	1.52
1	B	404	CFZ	C2'-C3'	-4.33	1.46	1.52
1	A	234	CFZ	C2'-C3'	-4.33	1.46	1.52
1	B	417	CFZ	C2'-C3'	-4.33	1.46	1.52
1	A	404	CFZ	C2'-C3'	-4.33	1.46	1.52
1	A	351	CFZ	C2'-C3'	-4.33	1.46	1.52
1	A	378	CFZ	C2'-C3'	-4.33	1.46	1.52
1	B	67	CFZ	C2'-C3'	-4.33	1.46	1.52
1	B	212	CFZ	C2'-C3'	-4.32	1.46	1.52
1	A	543	CFZ	C2'-C3'	-4.32	1.46	1.52
1	A	25	CFZ	C2'-C3'	-4.32	1.46	1.52
1	A	201	CFZ	C2'-C3'	-4.32	1.46	1.52
1	B	34	CFZ	C2'-C3'	-4.32	1.46	1.52
1	A	373	CFZ	C2'-C3'	-4.31	1.46	1.52
1	B	418	CFZ	C2'-C3'	-4.31	1.46	1.52
1	A	473	CFZ	C2'-C3'	-4.31	1.46	1.52
1	B	632	CFZ	C2'-C3'	-4.31	1.46	1.52
1	B	625	CFZ	C2'-C3'	-4.31	1.46	1.52
1	B	103	CFZ	C2'-C3'	-4.31	1.46	1.52
1	B	576	CFZ	C2'-C3'	-4.31	1.46	1.52
1	B	620	CFZ	C2'-C3'	-4.31	1.46	1.52
1	A	574	CFZ	C2'-C3'	-4.31	1.46	1.52
1	A	212	CFZ	C2'-C3'	-4.30	1.46	1.52
1	B	254	CFZ	C2'-C3'	-4.30	1.46	1.52
1	B	268	CFZ	C2'-C3'	-4.30	1.46	1.52
1	A	111	CFZ	C2'-C3'	-4.30	1.46	1.52
1	B	664	CFZ	C2'-C3'	-4.30	1.46	1.52
1	A	632	CFZ	C2'-C3'	-4.30	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	315	CFZ	C2'-C3'	-4.30	1.46	1.52
1	A	232	CFZ	C2'-C3'	-4.29	1.46	1.52
1	B	234	CFZ	C2'-C3'	-4.29	1.46	1.52
1	A	383	CFZ	C2'-C3'	-4.29	1.46	1.52
1	A	161	CFZ	C2'-C3'	-4.29	1.46	1.52
1	B	161	CFZ	C2'-C3'	-4.29	1.46	1.52
1	A	556	CFZ	C2'-C3'	-4.29	1.46	1.52
1	A	96	CFZ	C2'-C3'	-4.29	1.46	1.52
1	A	620	CFZ	C2'-C3'	-4.29	1.46	1.52
1	A	103	CFZ	C2'-C3'	-4.29	1.46	1.52
1	A	631	CFZ	C2'-C3'	-4.29	1.46	1.52
1	B	610	CFZ	C2'-C3'	-4.28	1.46	1.52
1	A	173	CFZ	C2'-C3'	-4.28	1.46	1.52
1	B	362	CFZ	C2'-C3'	-4.27	1.46	1.52
1	A	469	CFZ	C2'-C3'	-4.27	1.46	1.52
1	A	144	CFZ	C2'-C3'	-4.27	1.46	1.52
1	B	173	CFZ	C2'-C3'	-4.27	1.46	1.52
1	B	469	CFZ	C2'-C3'	-4.27	1.46	1.52
1	A	26	CFZ	C2'-C3'	-4.26	1.46	1.52
1	A	114	CFZ	C2'-C3'	-4.26	1.46	1.52
1	A	268	CFZ	C2'-C3'	-4.26	1.46	1.52
1	B	583	CFZ	C2'-C3'	-4.26	1.46	1.52
1	B	360	CFZ	C2'-C3'	-4.26	1.46	1.52
1	A	492	CFZ	C2'-C3'	-4.26	1.46	1.52
1	A	489	UFT	C5-C4	4.26	1.53	1.43
1	A	664	CFZ	C2'-C3'	-4.26	1.46	1.52
1	A	210	CFZ	C2'-C3'	-4.25	1.46	1.52
1	B	210	CFZ	C2'-C3'	-4.25	1.46	1.52
1	B	486	CFZ	C2'-C3'	-4.25	1.46	1.52
1	A	517	CFZ	C2'-C3'	-4.25	1.46	1.52
1	B	523	CFZ	C2'-C3'	-4.25	1.46	1.52
1	A	691	CFZ	C2'-C3'	-4.25	1.46	1.52
1	B	63	CFZ	C2'-C3'	-4.25	1.46	1.52
1	A	418	CFZ	C2'-C3'	-4.25	1.46	1.52
1	B	384	CFZ	C2'-C3'	-4.25	1.46	1.52
1	B	582	UFT	C5-C4	4.25	1.53	1.43
1	B	13	UFT	C5-C4	4.25	1.53	1.43
1	B	62	UFT	C5-C4	4.25	1.53	1.43
1	B	25	CFZ	C2'-C3'	-4.24	1.46	1.52
1	B	439	CFZ	C2'-C3'	-4.24	1.46	1.52
1	B	493	UFT	C2'-C3'	-4.24	1.46	1.52
1	A	143	UFT	C5-C4	4.24	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	518	CFZ	C2'-C3'	-4.24	1.46	1.52
1	A	309	UFT	C5-C4	4.24	1.53	1.43
1	B	214	UFT	C5-C4	4.24	1.53	1.43
1	A	86	UFT	C5-C4	4.24	1.53	1.43
1	A	444	CFZ	C2'-C3'	-4.23	1.46	1.52
1	A	69	UFT	C5-C4	4.23	1.53	1.43
1	A	438	CFZ	C2'-C3'	-4.23	1.46	1.52
1	A	498	CFZ	C2'-C3'	-4.23	1.46	1.52
1	B	69	UFT	C5-C4	4.23	1.53	1.43
1	A	336	UFT	C5-C4	4.23	1.53	1.43
1	B	117	CFZ	C2'-C3'	-4.23	1.46	1.52
1	A	241	CFZ	C2'-C3'	-4.23	1.46	1.52
1	B	358	UFT	C5-C4	4.23	1.53	1.43
1	B	88	UFT	C5-C4	4.23	1.53	1.43
1	A	504	UFT	C5-C4	4.23	1.53	1.43
1	A	200	UFT	C5-C4	4.23	1.53	1.43
1	A	106	UFT	C5-C4	4.23	1.53	1.43
1	A	116	UFT	C5-C4	4.23	1.53	1.43
1	B	431	UFT	C5-C4	4.23	1.53	1.43
1	A	14	UFT	C5-C4	4.23	1.53	1.43
1	A	190	UFT	C5-C4	4.23	1.53	1.43
1	B	215	UFT	C5-C4	4.23	1.53	1.43
1	B	114	CFZ	C2'-C3'	-4.23	1.46	1.52
1	B	308	CFZ	C2'-C3'	-4.23	1.46	1.52
1	B	485	UFT	C5-C4	4.23	1.53	1.43
1	A	690	UFT	C5-C4	4.23	1.53	1.43
1	A	153	UFT	C5-C4	4.23	1.53	1.43
1	A	663	UFT	C5-C4	4.23	1.53	1.43
1	A	94	UFT	C5-C4	4.23	1.53	1.43
1	B	636	UFT	C5-C4	4.23	1.53	1.43
1	B	182	UFT	C5-C4	4.23	1.53	1.43
1	A	202	UFT	C5-C4	4.23	1.53	1.43
1	B	296	UFT	C5-C4	4.23	1.53	1.43
1	B	398	UFT	C5-C4	4.22	1.53	1.43
1	B	153	UFT	C5-C4	4.22	1.53	1.43
1	A	160	UFT	C5-C4	4.22	1.53	1.43
1	B	301	UFT	C5-C4	4.22	1.53	1.43
1	B	519	UFT	C5-C4	4.22	1.53	1.43
1	B	61	UFT	C5-C4	4.22	1.53	1.43
1	A	662	UFT	C5-C4	4.22	1.53	1.43
1	B	74	UFT	C5-C4	4.22	1.53	1.43
1	A	666	UFT	C5-C4	4.22	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	UFT	C5-C4	4.22	1.53	1.43
1	A	590	UFT	C5-C4	4.22	1.53	1.43
1	A	629	UFT	C5-C4	4.22	1.53	1.43
1	B	347	UFT	C5-C4	4.22	1.53	1.43
1	B	637	CFZ	C2'-C3'	-4.22	1.46	1.52
1	A	559	UFT	C5-C4	4.22	1.53	1.43
1	B	666	UFT	C5-C4	4.22	1.53	1.43
1	A	155	UFT	C5-C4	4.22	1.53	1.43
1	A	696	UFT	C5-C4	4.22	1.53	1.43
1	A	117	CFZ	C2'-C3'	-4.22	1.46	1.52
1	B	502	UFT	C5-C4	4.22	1.53	1.43
1	A	417	CFZ	C2'-C3'	-4.22	1.46	1.52
1	A	583	CFZ	C2'-C3'	-4.22	1.46	1.52
1	A	493	UFT	C5-C4	4.22	1.53	1.43
1	A	430	UFT	C5-C4	4.22	1.53	1.43
1	B	635	UFT	C5-C4	4.22	1.53	1.43
1	A	182	UFT	C5-C4	4.22	1.53	1.43
1	A	296	UFT	C5-C4	4.22	1.53	1.43
1	A	365	UFT	C5-C4	4.22	1.53	1.43
1	A	582	UFT	C5-C4	4.22	1.53	1.43
1	A	720	UFT	C5-C4	4.22	1.53	1.43
1	B	98	UFT	C5-C4	4.22	1.53	1.43
1	B	352	UFT	C5-C4	4.22	1.53	1.43
1	B	609	UFT	C5-C4	4.22	1.53	1.43
1	B	144	CFZ	C2'-C3'	-4.22	1.46	1.52
1	B	465	CFZ	C2'-C3'	-4.22	1.46	1.52
1	B	163	UFT	C5-C4	4.22	1.53	1.43
1	A	59	UFT	C5-C4	4.22	1.53	1.43
1	B	241	CFZ	C2'-C3'	-4.22	1.46	1.52
1	B	498	CFZ	C2'-C3'	-4.22	1.46	1.52
1	B	556	CFZ	C2'-C3'	-4.22	1.46	1.52
1	A	88	UFT	C5-C4	4.22	1.53	1.43
1	A	245	UFT	C5-C4	4.22	1.53	1.43
1	B	438	CFZ	C2'-C3'	-4.21	1.46	1.52
1	A	637	CFZ	C2'-C3'	-4.21	1.46	1.52
1	A	197	UFT	C5-C4	4.21	1.53	1.43
1	A	689	UFT	C5-C4	4.21	1.53	1.43
1	A	89	UFT	C5-C4	4.21	1.53	1.43
1	A	217	UFT	C5-C4	4.21	1.53	1.43
1	A	283	UFT	C5-C4	4.21	1.53	1.43
1	A	170	UFT	C5-C4	4.21	1.53	1.43
1	B	581	UFT	C5-C4	4.21	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	CFZ	C2'-C3'	-4.21	1.46	1.52
1	B	691	CFZ	C2'-C3'	-4.21	1.46	1.52
1	B	116	UFT	C5-C4	4.21	1.53	1.43
1	A	63	CFZ	C2'-C3'	-4.21	1.46	1.52
1	A	554	UFT	C5-C4	4.21	1.53	1.43
1	A	97	UFT	C5-C4	4.21	1.53	1.43
1	A	115	UFT	C5-C4	4.21	1.53	1.43
1	A	142	UFT	C5-C4	4.21	1.53	1.43
1	A	403	UFT	C5-C4	4.21	1.53	1.43
1	A	328	CFZ	C2'-C3'	-4.21	1.46	1.52
1	A	251	UFT	C5-C4	4.21	1.53	1.43
1	A	500	UFT	C5-C4	4.21	1.53	1.43
1	A	502	UFT	C5-C4	4.21	1.53	1.43
1	A	653	UFT	C5-C4	4.21	1.53	1.43
1	B	328	CFZ	C2'-C3'	-4.21	1.46	1.52
1	B	353	CFZ	C2'-C3'	-4.21	1.46	1.52
1	A	126	UFT	C5-C4	4.21	1.52	1.43
1	A	301	UFT	C5-C4	4.21	1.52	1.43
1	B	434	UFT	C5-C4	4.21	1.52	1.43
1	B	530	UFT	C5-C4	4.21	1.52	1.43
1	B	338	CFZ	C2'-C3'	-4.21	1.46	1.52
1	B	504	UFT	C5-C4	4.21	1.52	1.43
1	A	154	UFT	C5-C4	4.21	1.52	1.43
1	A	214	UFT	C5-C4	4.21	1.52	1.43
1	B	607	UFT	C5-C4	4.21	1.52	1.43
1	B	687	UFT	C5-C4	4.21	1.52	1.43
1	B	90	CFZ	C2'-C3'	-4.21	1.46	1.52
1	B	160	UFT	C5-C4	4.21	1.52	1.43
1	A	434	UFT	C5-C4	4.21	1.52	1.43
1	B	115	UFT	C5-C4	4.21	1.52	1.43
1	A	61	UFT	C5-C4	4.21	1.52	1.43
1	A	610	CFZ	C2'-C3'	-4.21	1.46	1.52
1	B	170	UFT	C5-C4	4.21	1.52	1.43
1	B	322	UFT	C5-C4	4.21	1.52	1.43
1	B	233	UFT	C5-C4	4.21	1.52	1.43
1	A	366	UFT	C5-C4	4.21	1.52	1.43
1	B	265	UFT	C5-C4	4.21	1.52	1.43
1	B	559	UFT	C5-C4	4.21	1.52	1.43
1	A	695	UFT	C5-C4	4.21	1.52	1.43
1	A	233	UFT	C5-C4	4.21	1.52	1.43
1	B	309	UFT	C5-C4	4.21	1.52	1.43
1	B	142	UFT	C5-C4	4.20	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	UFT	C5-C4	4.20	1.52	1.43
1	B	126	UFT	C5-C4	4.20	1.52	1.43
1	B	141	UFT	C5-C4	4.20	1.52	1.43
1	B	204	UFT	C5-C4	4.20	1.52	1.43
1	B	690	UFT	C5-C4	4.20	1.52	1.43
1	B	55	UFT	C5-C4	4.20	1.52	1.43
1	A	179	UFT	C5-C4	4.20	1.52	1.43
1	B	19	UFT	C5-C4	4.20	1.52	1.43
1	A	621	UFT	C5-C4	4.20	1.52	1.43
1	A	389	UFT	C5-C4	4.20	1.52	1.43
1	B	464	UFT	C5-C4	4.20	1.52	1.43
1	B	42	UFT	C2'-C3'	-4.20	1.46	1.52
1	B	282	CFZ	C2'-C3'	-4.20	1.46	1.52
1	B	229	UFT	C5-C4	4.20	1.52	1.43
1	A	60	UFT	C5-C4	4.20	1.52	1.43
1	B	60	UFT	C5-C4	4.20	1.52	1.43
1	A	593	UFT	C5-C4	4.20	1.52	1.43
1	B	695	UFT	C5-C4	4.20	1.52	1.43
1	B	33	UFT	C5-C4	4.20	1.52	1.43
1	A	55	UFT	C5-C4	4.20	1.52	1.43
1	B	197	UFT	C5-C4	4.20	1.52	1.43
1	A	19	UFT	C5-C4	4.20	1.52	1.43
1	B	367	UFT	C5-C4	4.20	1.52	1.43
1	A	137	UFT	C5-C4	4.20	1.52	1.43
1	B	155	UFT	C5-C4	4.20	1.52	1.43
1	B	403	UFT	C5-C4	4.20	1.52	1.43
1	B	500	UFT	C5-C4	4.20	1.52	1.43
1	B	108	UFT	C2'-C3'	-4.20	1.46	1.52
1	A	13	UFT	C5-C4	4.20	1.52	1.43
1	B	283	UFT	C5-C4	4.20	1.52	1.43
1	B	336	UFT	C5-C4	4.20	1.52	1.43
1	A	367	UFT	C5-C4	4.20	1.52	1.43
1	A	703	UFT	C5-C4	4.20	1.52	1.43
1	A	84	UFT	C5-C4	4.20	1.52	1.43
1	B	542	UFT	C5-C4	4.20	1.52	1.43
1	A	32	UFT	C5-C4	4.20	1.52	1.43
1	B	143	UFT	C5-C4	4.20	1.52	1.43
1	B	154	UFT	C5-C4	4.20	1.52	1.43
1	A	635	UFT	C5-C4	4.20	1.52	1.43
1	B	708	UFT	C5-C4	4.20	1.52	1.43
1	A	509	UFT	C5-C4	4.20	1.52	1.43
1	A	719	UFT	C5-C4	4.20	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	UFT	C5-C4	4.20	1.52	1.43
1	A	329	UFT	C5-C4	4.20	1.52	1.43
1	A	48	UFT	C5-C4	4.20	1.52	1.43
1	B	534	UFT	C5-C4	4.20	1.52	1.43
1	B	555	UFT	C5-C4	4.20	1.52	1.43
1	A	360	CFZ	C2'-C3'	-4.20	1.46	1.52
1	B	200	UFT	C5-C4	4.20	1.52	1.43
1	B	359	UFT	C5-C4	4.20	1.52	1.43
1	A	485	UFT	C5-C4	4.20	1.52	1.43
1	B	217	UFT	C5-C4	4.20	1.52	1.43
1	A	282	CFZ	C2'-C3'	-4.19	1.46	1.52
1	A	204	UFT	C5-C4	4.19	1.52	1.43
1	A	344	UFT	C5-C4	4.19	1.52	1.43
1	B	472	UFT	C5-C4	4.19	1.52	1.43
1	B	499	UFT	C5-C4	4.19	1.52	1.43
1	B	71	UFT	C5-C4	4.19	1.52	1.43
1	B	366	UFT	C5-C4	4.19	1.52	1.43
1	B	365	UFT	C5-C4	4.19	1.52	1.43
1	B	466	UFT	C5-C4	4.19	1.52	1.43
1	B	59	UFT	C5-C4	4.19	1.52	1.43
1	B	473	CFZ	C2'-C3'	-4.19	1.46	1.52
1	B	536	CFZ	C2'-C3'	-4.19	1.46	1.52
1	B	94	UFT	C5-C4	4.19	1.52	1.43
1	A	708	UFT	C5-C4	4.19	1.52	1.43
1	A	266	UFT	C5-C4	4.19	1.52	1.43
1	B	208	UFT	C5-C4	4.19	1.52	1.43
1	B	629	UFT	C5-C4	4.19	1.52	1.43
1	A	305	UFT	C5-C4	4.19	1.52	1.43
1	B	421	UFT	C5-C4	4.19	1.52	1.43
1	A	608	UFT	C5-C4	4.19	1.52	1.43
1	B	593	UFT	C5-C4	4.19	1.52	1.43
1	A	353	CFZ	C2'-C3'	-4.19	1.46	1.52
1	A	50	UFT	C5-C4	4.19	1.52	1.43
1	B	84	UFT	C5-C4	4.19	1.52	1.43
1	A	334	UFT	C5-C4	4.19	1.52	1.43
1	A	163	UFT	C5-C4	4.19	1.52	1.43
1	A	308	CFZ	C2'-C3'	-4.19	1.46	1.52
1	A	609	UFT	C5-C4	4.19	1.52	1.43
1	A	33	UFT	C5-C4	4.19	1.52	1.43
1	A	42	UFT	C5-C4	4.19	1.52	1.43
1	A	636	UFT	C5-C4	4.19	1.52	1.43
1	B	101	UFT	C5-C4	4.19	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	UFT	C5-C4	4.19	1.52	1.43
1	B	633	UFT	C5-C4	4.19	1.52	1.43
1	B	513	UFT	C2'-C3'	-4.19	1.46	1.52
1	B	137	UFT	C5-C4	4.19	1.52	1.43
1	A	141	UFT	C5-C4	4.19	1.52	1.43
1	A	437	UFT	C5-C4	4.19	1.52	1.43
1	B	662	UFT	C5-C4	4.19	1.52	1.43
1	B	494	CFZ	C2-N3	4.19	1.44	1.36
1	A	701	UFT	C5-C4	4.19	1.52	1.43
1	B	11	UFT	C5-C4	4.19	1.52	1.43
1	A	92	UFT	C5-C4	4.19	1.52	1.43
1	A	350	UFT	C5-C4	4.19	1.52	1.43
1	A	581	UFT	C5-C4	4.19	1.52	1.43
1	B	696	UFT	C5-C4	4.19	1.52	1.43
1	B	97	UFT	C5-C4	4.18	1.52	1.43
1	A	687	UFT	C5-C4	4.18	1.52	1.43
1	B	14	UFT	C5-C4	4.18	1.52	1.43
1	A	352	UFT	C5-C4	4.18	1.52	1.43
1	A	413	UFT	C5-C4	4.18	1.52	1.43
1	A	618	UFT	C5-C4	4.18	1.52	1.43
1	B	554	UFT	C5-C4	4.18	1.52	1.43
1	B	653	UFT	C5-C4	4.18	1.52	1.43
1	B	169	UFT	C5-C4	4.18	1.52	1.43
1	A	361	UFT	C5-C4	4.18	1.52	1.43
1	B	423	UFT	C5-C4	4.18	1.52	1.43
1	A	466	UFT	C5-C4	4.18	1.52	1.43
1	B	606	UFT	C5-C4	4.18	1.52	1.43
1	A	71	UFT	C5-C4	4.18	1.52	1.43
1	B	389	UFT	C5-C4	4.18	1.52	1.43
1	B	437	UFT	C5-C4	4.18	1.52	1.43
1	B	590	UFT	C5-C4	4.18	1.52	1.43
1	A	8	UFT	C5-C4	4.18	1.52	1.43
1	B	89	UFT	C5-C4	4.18	1.52	1.43
1	A	208	UFT	C5-C4	4.18	1.52	1.43
1	B	270	UFT	C5-C4	4.18	1.52	1.43
1	A	398	UFT	C5-C4	4.18	1.52	1.43
1	A	555	UFT	C5-C4	4.18	1.52	1.43
1	A	673	UFT	C5-C4	4.18	1.52	1.43
1	B	293	UFT	C5-C4	4.18	1.52	1.43
1	B	618	UFT	C5-C4	4.18	1.52	1.43
1	A	712	UFT	C5-C4	4.18	1.52	1.43
1	B	251	UFT	C5-C4	4.18	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	UFT	C5-C4	4.18	1.52	1.43
1	A	534	UFT	C5-C4	4.18	1.52	1.43
1	B	545	UFT	C5-C4	4.18	1.52	1.43
1	B	621	UFT	C5-C4	4.18	1.52	1.43
1	B	646	UFT	C5-C4	4.18	1.52	1.43
1	A	175	UFT	C5-C4	4.18	1.52	1.43
1	B	402	UFT	C5-C4	4.18	1.52	1.43
1	B	456	UFT	C5-C4	4.18	1.52	1.43
1	A	669	UFT	C5-C4	4.18	1.52	1.43
1	A	112	UFT	C5-C4	4.18	1.52	1.43
1	B	202	UFT	C5-C4	4.18	1.52	1.43
1	A	347	UFT	C5-C4	4.18	1.52	1.43
1	A	606	UFT	C5-C4	4.18	1.52	1.43
1	A	684	UFT	C5-C4	4.18	1.52	1.43
1	B	179	UFT	C5-C4	4.18	1.52	1.43
1	A	549	UFT	C5-C4	4.18	1.52	1.43
1	B	720	UFT	C5-C4	4.18	1.52	1.43
1	B	15	CFZ	C2'-C3'	-4.18	1.46	1.52
1	B	266	UFT	C5-C4	4.18	1.52	1.43
1	B	460	UFT	C5-C4	4.18	1.52	1.43
1	A	545	UFT	C5-C4	4.18	1.52	1.43
1	B	628	UFT	C5-C4	4.18	1.52	1.43
1	A	174	UFT	C5-C4	4.18	1.52	1.43
1	A	260	UFT	C5-C4	4.18	1.52	1.43
1	B	106	UFT	C5-C4	4.18	1.52	1.43
1	A	456	UFT	C5-C4	4.18	1.52	1.43
1	A	542	UFT	C5-C4	4.18	1.52	1.43
1	A	544	UFT	C5-C4	4.18	1.52	1.43
1	B	549	UFT	C5-C4	4.18	1.52	1.43
1	B	701	UFT	C5-C4	4.18	1.52	1.43
1	A	74	UFT	C5-C4	4.18	1.52	1.43
1	B	175	UFT	C5-C4	4.18	1.52	1.43
1	A	423	UFT	C5-C4	4.18	1.52	1.43
1	B	459	CFZ	C2'-C3'	-4.17	1.46	1.52
1	A	460	UFT	C5-C4	4.17	1.52	1.43
1	B	608	UFT	C5-C4	4.17	1.52	1.43
1	B	663	UFT	C5-C4	4.17	1.52	1.43
1	B	260	UFT	C5-C4	4.17	1.52	1.43
1	A	519	UFT	C5-C4	4.17	1.52	1.43
1	A	62	UFT	C5-C4	4.17	1.52	1.43
1	B	305	UFT	C5-C4	4.17	1.52	1.43
1	A	377	UFT	C5-C4	4.17	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	656	UFT	C5-C4	4.17	1.52	1.43
1	B	245	UFT	C2'-C3'	-4.17	1.46	1.52
1	B	430	UFT	C5-C4	4.17	1.52	1.43
1	B	8	UFT	C5-C4	4.17	1.52	1.43
1	A	535	UFT	C2'-C3'	-4.17	1.46	1.52
1	A	472	UFT	C5-C4	4.17	1.52	1.43
1	B	192	UFT	C5-C4	4.17	1.52	1.43
1	A	135	UFT	C5-C4	4.17	1.52	1.43
1	B	334	UFT	C5-C4	4.17	1.52	1.43
1	A	447	UFT	C5-C4	4.17	1.52	1.43
1	B	577	UFT	C5-C4	4.17	1.52	1.43
1	A	293	UFT	C5-C4	4.17	1.52	1.43
1	A	577	UFT	C5-C4	4.17	1.52	1.43
1	B	602	UFT	C5-C4	4.17	1.52	1.43
1	A	465	CFZ	C2'-C3'	-4.17	1.46	1.52
1	B	48	UFT	C5-C4	4.17	1.52	1.43
1	A	530	UFT	C5-C4	4.17	1.52	1.43
1	A	464	UFT	C5-C4	4.17	1.52	1.43
1	A	471	UFT	C5-C4	4.17	1.52	1.43
1	B	509	UFT	C5-C4	4.17	1.52	1.43
1	A	607	UFT	C5-C4	4.17	1.52	1.43
1	A	90	CFZ	C2'-C3'	-4.17	1.46	1.52
1	A	108	UFT	C5-C4	4.17	1.52	1.43
1	B	689	UFT	C5-C4	4.17	1.52	1.43
1	A	313	UFT	C5-C4	4.16	1.52	1.43
1	B	535	UFT	C5-C4	4.16	1.52	1.43
1	A	656	UFT	C5-C4	4.16	1.52	1.43
1	B	684	UFT	C5-C4	4.16	1.52	1.43
1	B	344	UFT	C5-C4	4.16	1.52	1.43
1	A	633	UFT	C5-C4	4.16	1.52	1.43
1	B	712	UFT	C5-C4	4.16	1.52	1.43
1	B	232	CFZ	C2'-C3'	-4.16	1.46	1.52
1	B	447	UFT	C5-C4	4.16	1.52	1.43
1	A	11	UFT	C5-C4	4.16	1.52	1.43
1	A	229	UFT	C5-C4	4.16	1.52	1.43
1	A	108	UFT	C2'-C3'	-4.16	1.46	1.52
1	A	446	CFZ	C2'-C3'	-4.16	1.46	1.52
1	A	169	UFT	C5-C4	4.16	1.52	1.43
1	A	101	UFT	C5-C4	4.16	1.52	1.43
1	B	86	UFT	C5-C4	4.16	1.52	1.43
1	B	669	UFT	C5-C4	4.16	1.52	1.43
1	B	50	UFT	C5-C4	4.16	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	313	UFT	C5-C4	4.16	1.52	1.43
1	A	499	UFT	C5-C4	4.16	1.52	1.43
1	B	361	UFT	C5-C4	4.16	1.52	1.43
1	A	628	UFT	C5-C4	4.16	1.52	1.43
1	A	602	UFT	C5-C4	4.16	1.52	1.43
1	A	171	CFZ	C2'-C3'	-4.16	1.46	1.52
1	A	44	UFT	C5-C4	4.16	1.52	1.43
1	B	135	UFT	C5-C4	4.16	1.52	1.43
1	B	703	UFT	C5-C4	4.16	1.52	1.43
1	B	108	UFT	C5-C4	4.16	1.52	1.43
1	A	192	UFT	C5-C4	4.16	1.52	1.43
1	A	646	UFT	C5-C4	4.16	1.52	1.43
1	A	503	UFT	C5-C4	4.15	1.52	1.43
1	B	329	UFT	C5-C4	4.15	1.52	1.43
1	B	80	UFT	C5-C4	4.15	1.52	1.43
1	A	440	CFZ	C2'-C3'	-4.15	1.46	1.52
1	B	471	UFT	C5-C4	4.15	1.52	1.43
1	B	571	UFT	C5-C4	4.15	1.52	1.43
1	A	196	UFT	C5-C4	4.15	1.52	1.43
1	B	174	UFT	C5-C4	4.15	1.52	1.43
1	B	216	UFT	C5-C4	4.15	1.52	1.43
1	A	571	UFT	C5-C4	4.15	1.52	1.43
1	A	513	UFT	C5-C4	4.15	1.52	1.43
1	B	245	UFT	C5-C4	4.15	1.52	1.43
1	B	524	UFT	C5-C4	4.15	1.52	1.43
1	B	96	CFZ	C2'-C3'	-4.15	1.47	1.52
1	A	140	CFZ	C2'-C3'	-4.15	1.47	1.52
1	B	171	CFZ	C2'-C3'	-4.14	1.47	1.52
1	B	377	UFT	C5-C4	4.14	1.52	1.43
1	A	513	UFT	C2'-C3'	-4.14	1.47	1.52
1	B	112	UFT	C5-C4	4.14	1.52	1.43
1	B	432	UFT	C5-C4	4.14	1.52	1.43
1	B	42	UFT	C5-C4	4.14	1.52	1.43
1	B	544	UFT	C5-C4	4.14	1.52	1.43
1	A	524	UFT	C5-C4	4.14	1.52	1.43
1	A	535	UFT	C5-C4	4.14	1.52	1.43
1	A	421	UFT	C5-C4	4.14	1.52	1.43
1	B	92	UFT	C5-C4	4.14	1.52	1.43
1	B	196	UFT	C5-C4	4.14	1.52	1.43
1	B	32	UFT	C5-C4	4.13	1.52	1.43
1	A	481	UFT	C5-C4	4.13	1.52	1.43
1	B	659	UFT	C5-C4	4.13	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	UFT	C5-C4	4.13	1.52	1.43
1	B	513	UFT	C5-C4	4.13	1.52	1.43
1	B	673	UFT	C5-C4	4.13	1.52	1.43
1	B	321	CFZ	C2'-C3'	-4.13	1.47	1.52
1	A	676	UFT	C5-C4	4.13	1.52	1.43
1	B	489	UFT	C5-C4	4.13	1.52	1.43
1	A	432	UFT	C5-C4	4.13	1.52	1.43
1	B	10	CFZ	C2'-C3'	-4.13	1.47	1.52
1	A	367	UFT	C2'-C3'	-4.13	1.47	1.52
1	A	322	UFT	C5-C4	4.13	1.52	1.43
1	B	676	UFT	C5-C4	4.13	1.52	1.43
1	A	98	UFT	C5-C4	4.12	1.52	1.43
1	A	105	UFT	C5-C4	4.12	1.52	1.43
1	A	75	CFZ	C2'-C3'	-4.12	1.47	1.52
1	A	358	UFT	C5-C4	4.12	1.52	1.43
1	A	15	CFZ	C2'-C3'	-4.12	1.47	1.52
1	B	246	CFZ	C2-N3	4.12	1.44	1.36
1	A	315	CFZ	C2-N3	4.11	1.44	1.36
1	B	43	UFT	C5-C4	4.11	1.52	1.43
1	A	564	CFZ	C2-N3	4.11	1.44	1.36
1	A	313	UFT	C2'-C3'	-4.11	1.47	1.52
1	B	140	CFZ	C2'-C3'	-4.11	1.47	1.52
1	B	481	UFT	C5-C4	4.11	1.52	1.43
1	A	43	UFT	C5-C4	4.11	1.52	1.43
1	B	105	UFT	C5-C4	4.11	1.52	1.43
1	A	684	UFT	C2'-C3'	-4.11	1.47	1.52
1	A	574	CFZ	C2-N3	4.10	1.44	1.36
1	A	359	UFT	C5-C4	4.10	1.52	1.43
1	A	260	UFT	C2'-C3'	-4.10	1.47	1.52
1	A	42	UFT	C2'-C3'	-4.10	1.47	1.52
1	B	564	CFZ	C2-N3	4.10	1.44	1.36
1	A	659	UFT	C5-C4	4.10	1.52	1.43
1	A	96	CFZ	C2-N3	4.10	1.44	1.36
1	B	219	CFZ	C2-N3	4.10	1.44	1.36
1	B	44	UFT	C5-C4	4.10	1.52	1.43
1	B	358	UFT	C2'-C3'	-4.10	1.47	1.52
1	B	684	UFT	C2'-C3'	-4.10	1.47	1.52
1	B	647	CFZ	C2-N3	4.09	1.44	1.36
1	A	328	CFZ	C2-N3	4.09	1.44	1.36
1	B	260	UFT	C2'-C3'	-4.09	1.47	1.52
1	B	719	UFT	C5-C4	4.09	1.52	1.43
1	B	216	UFT	C2'-C3'	-4.09	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	CFZ	C2-N3	4.09	1.44	1.36
1	B	173	CFZ	C2-N3	4.09	1.44	1.36
1	A	458	CFZ	C2-N3	4.09	1.44	1.36
1	A	548	CFZ	C2-N3	4.09	1.44	1.36
1	A	530	UFT	C2'-C3'	-4.09	1.47	1.52
1	B	426	CFZ	C2-N3	4.09	1.44	1.36
1	A	173	CFZ	C2-N3	4.09	1.44	1.36
1	A	298	CFZ	C2-N3	4.09	1.44	1.36
1	B	315	CFZ	C2-N3	4.09	1.44	1.36
1	B	518	CFZ	C2-N3	4.09	1.44	1.36
1	A	455	CFZ	C2-N3	4.08	1.44	1.36
1	A	647	CFZ	C2-N3	4.08	1.44	1.36
1	A	506	CFZ	C2-N3	4.08	1.44	1.36
1	A	550	CFZ	C2-N3	4.08	1.44	1.36
1	B	218	CFZ	C2'-C3'	-4.08	1.47	1.52
1	B	304	CFZ	C2-N3	4.08	1.44	1.36
1	A	308	CFZ	C2-N3	4.08	1.44	1.36
1	B	540	CFZ	C2-N3	4.08	1.44	1.36
1	A	511	CFZ	C2-N3	4.08	1.44	1.36
1	B	667	CFZ	C2-N3	4.08	1.44	1.36
1	B	698	CFZ	C2-N3	4.08	1.44	1.36
1	A	10	CFZ	C2-N3	4.08	1.44	1.36
1	B	550	CFZ	C2-N3	4.08	1.44	1.36
1	A	206	CFZ	C2-N3	4.08	1.44	1.36
1	B	372	CFZ	C2-N3	4.08	1.44	1.36
1	B	446	CFZ	C2'-C3'	-4.08	1.47	1.52
1	B	114	CFZ	C2-N3	4.08	1.44	1.36
1	A	338	CFZ	C2-N3	4.08	1.44	1.36
1	A	474	CFZ	C2-N3	4.08	1.44	1.36
1	A	679	CFZ	C2-N3	4.08	1.44	1.36
1	A	459	CFZ	C2-N3	4.08	1.44	1.36
1	B	631	CFZ	C2-N3	4.08	1.44	1.36
1	B	285	CFZ	C2-N3	4.08	1.44	1.36
1	A	382	CFZ	C2-N3	4.08	1.44	1.36
1	A	492	CFZ	C2-N3	4.08	1.44	1.36
1	B	517	CFZ	C2-N3	4.08	1.44	1.36
1	A	540	CFZ	C2-N3	4.08	1.44	1.36
1	A	498	CFZ	C2-N3	4.08	1.44	1.36
1	B	600	CFZ	C2-N3	4.08	1.44	1.36
1	B	218	CFZ	C2-N3	4.08	1.44	1.36
1	A	120	CFZ	C2-N3	4.08	1.44	1.36
1	B	212	CFZ	C2-N3	4.08	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	CFZ	C2-N3	4.08	1.44	1.36
1	B	498	CFZ	C2-N3	4.08	1.44	1.36
1	A	139	CFZ	C2-N3	4.07	1.44	1.36
1	B	316	CFZ	C2-N3	4.07	1.44	1.36
1	A	568	CFZ	C2-N3	4.07	1.44	1.36
1	A	316	CFZ	C2-N3	4.07	1.44	1.36
1	B	592	CFZ	C2-N3	4.07	1.44	1.36
1	B	206	CFZ	C2-N3	4.07	1.44	1.36
1	A	161	CFZ	C2-N3	4.07	1.44	1.36
1	A	242	CFZ	C2-N3	4.07	1.44	1.36
1	B	469	CFZ	C2-N3	4.07	1.44	1.36
1	A	465	CFZ	C2-N3	4.07	1.44	1.36
1	A	637	CFZ	C2-N3	4.07	1.44	1.36
1	B	179	UFT	C2'-C3'	-4.07	1.47	1.52
1	B	76	CFZ	C2-N3	4.07	1.44	1.36
1	B	425	CFZ	C2-N3	4.07	1.44	1.36
1	B	576	CFZ	C2-N3	4.07	1.44	1.36
1	A	33	UFT	C2'-C3'	-4.07	1.47	1.52
1	B	57	CFZ	C2-N3	4.07	1.44	1.36
1	A	67	CFZ	C2-N3	4.07	1.44	1.36
1	A	517	CFZ	C2-N3	4.07	1.44	1.36
1	B	679	CFZ	C2-N3	4.07	1.44	1.36
1	A	698	CFZ	C2-N3	4.07	1.44	1.36
1	A	459	CFZ	C2'-C3'	-4.07	1.47	1.52
1	A	603	CFZ	C2-N3	4.07	1.44	1.36
1	A	57	CFZ	C2-N3	4.07	1.44	1.36
1	A	512	CFZ	C2-N3	4.07	1.44	1.36
1	B	583	CFZ	C2-N3	4.07	1.44	1.36
1	B	652	CFZ	C2-N3	4.07	1.44	1.36
1	B	603	CFZ	C2-N3	4.07	1.44	1.36
1	B	651	CFZ	C2-N3	4.07	1.44	1.36
1	B	383	CFZ	C2'-C3'	-4.07	1.47	1.52
1	A	241	CFZ	C2-N3	4.07	1.44	1.36
1	A	405	CFZ	C2-N3	4.07	1.44	1.36
1	A	625	CFZ	C2-N3	4.07	1.44	1.36
1	B	103	CFZ	C2-N3	4.07	1.44	1.36
1	A	373	CFZ	C2-N3	4.07	1.44	1.36
1	B	399	CFZ	C2-N3	4.07	1.44	1.36
1	A	156	CFZ	C2-N3	4.07	1.44	1.36
1	A	279	CFZ	C2-N3	4.07	1.44	1.36
1	B	335	CFZ	C2-N3	4.07	1.44	1.36
1	B	338	CFZ	C2-N3	4.07	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	CFZ	C2'-C3'	-4.07	1.47	1.52
1	B	298	CFZ	C2-N3	4.07	1.44	1.36
1	B	693	CFZ	C2-N3	4.07	1.44	1.36
1	B	465	CFZ	C2-N3	4.07	1.44	1.36
1	B	139	CFZ	C2-N3	4.06	1.44	1.36
1	A	558	CFZ	C2-N3	4.06	1.44	1.36
1	A	124	CFZ	C2-N3	4.06	1.44	1.36
1	B	268	CFZ	C2-N3	4.06	1.44	1.36
1	A	438	CFZ	C2-N3	4.06	1.44	1.36
1	A	610	CFZ	C2-N3	4.06	1.44	1.36
1	A	655	CFZ	C2-N3	4.06	1.44	1.36
1	A	151	CFZ	C2-N3	4.06	1.44	1.36
1	B	355	CFZ	C2-N3	4.06	1.44	1.36
1	B	362	CFZ	C2-N3	4.06	1.44	1.36
1	B	72	CFZ	C2-N3	4.06	1.44	1.36
1	A	114	CFZ	C2-N3	4.06	1.44	1.36
1	A	372	CFZ	C2-N3	4.06	1.44	1.36
1	A	417	CFZ	C2-N3	4.06	1.44	1.36
1	B	63	CFZ	C2-N3	4.06	1.44	1.36
1	B	254	CFZ	C2-N3	4.06	1.44	1.36
1	B	279	CFZ	C2-N3	4.06	1.44	1.36
1	B	282	CFZ	C2-N3	4.06	1.44	1.36
1	A	639	CFZ	C2-N3	4.06	1.44	1.36
1	B	704	CFZ	C2-N3	4.06	1.44	1.36
1	B	39	CFZ	C2-N3	4.06	1.44	1.36
1	A	355	CFZ	C2-N3	4.06	1.44	1.36
1	A	406	CFZ	C2-N3	4.06	1.44	1.36
1	B	441	CFZ	C2-N3	4.06	1.44	1.36
1	B	161	CFZ	C2-N3	4.06	1.44	1.36
1	B	249	CFZ	C2-N3	4.06	1.44	1.36
1	A	358	UFT	C2'-C3'	-4.06	1.47	1.52
1	A	209	CFZ	C2-N3	4.06	1.44	1.36
1	A	218	CFZ	C2-N3	4.06	1.44	1.36
1	A	325	CFZ	C2-N3	4.06	1.44	1.36
1	B	446	CFZ	C2-N3	4.06	1.44	1.36
1	B	511	CFZ	C2-N3	4.06	1.44	1.36
1	B	308	CFZ	C2-N3	4.06	1.44	1.36
1	B	370	CFZ	C2-N3	4.06	1.44	1.36
1	A	131	CFZ	C2-N3	4.06	1.44	1.36
1	A	232	CFZ	C2-N3	4.06	1.44	1.36
1	A	369	CFZ	C2-N3	4.06	1.44	1.36
1	B	251	UFT	C2'-C3'	-4.06	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	CFZ	C2-N3	4.06	1.44	1.36
1	B	110	CFZ	C2-N3	4.06	1.44	1.36
1	B	323	CFZ	C2-N3	4.06	1.44	1.36
1	B	124	CFZ	C2-N3	4.06	1.44	1.36
1	A	171	CFZ	C2-N3	4.06	1.44	1.36
1	A	446	CFZ	C2-N3	4.06	1.44	1.36
1	A	283	UFT	C2'-C3'	-4.06	1.47	1.52
1	B	242	CFZ	C2-N3	4.06	1.44	1.36
1	A	214	UFT	C2'-C3'	-4.06	1.47	1.52
1	B	149	CFZ	C2-N3	4.06	1.44	1.36
1	B	486	CFZ	C2-N3	4.06	1.44	1.36
1	A	365	UFT	C2'-C3'	-4.06	1.47	1.52
1	B	703	UFT	C2'-C3'	-4.06	1.47	1.52
1	A	254	CFZ	C2-N3	4.05	1.44	1.36
1	A	440	CFZ	C2-N3	4.05	1.44	1.36
1	B	655	CFZ	C2-N3	4.05	1.44	1.36
1	A	302	UFT	C5-C4	4.05	1.52	1.43
1	A	323	CFZ	C2-N3	4.05	1.44	1.36
1	B	682	CFZ	C2-N3	4.05	1.44	1.36
1	A	15	CFZ	C2-N3	4.05	1.44	1.36
1	B	373	CFZ	C2-N3	4.05	1.44	1.36
1	A	426	CFZ	C2-N3	4.05	1.44	1.36
1	B	25	CFZ	C2-N3	4.05	1.44	1.36
1	A	565	CFZ	C2-N3	4.05	1.44	1.36
1	B	657	CFZ	C2-N3	4.05	1.44	1.36
1	A	491	CFZ	C2-N3	4.05	1.44	1.36
1	A	413	UFT	C2'-C3'	-4.05	1.47	1.52
1	B	568	CFZ	C2-N3	4.05	1.44	1.36
1	A	632	CFZ	C2-N3	4.05	1.44	1.36
1	A	117	CFZ	C2-N3	4.05	1.44	1.36
1	B	411	CFZ	C2-N3	4.05	1.44	1.36
1	B	558	CFZ	C2-N3	4.05	1.44	1.36
1	A	304	CFZ	C2-N3	4.05	1.44	1.36
1	B	439	CFZ	C2-N3	4.05	1.44	1.36
1	B	474	CFZ	C2-N3	4.05	1.44	1.36
1	A	436	CFZ	C2-N3	4.05	1.44	1.36
1	A	444	CFZ	C2-N3	4.05	1.44	1.36
1	B	551	CFZ	C2-N3	4.05	1.44	1.36
1	A	587	CFZ	C2-N3	4.05	1.44	1.36
1	A	667	CFZ	C2-N3	4.05	1.44	1.36
1	B	79	CFZ	C2-N3	4.05	1.44	1.36
1	A	604	CFZ	C2-N3	4.05	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	CFZ	C2-N3	4.05	1.44	1.36
1	B	383	CFZ	C2-N3	4.05	1.44	1.36
1	B	459	CFZ	C2-N3	4.05	1.44	1.36
1	A	201	CFZ	C2-N3	4.05	1.44	1.36
1	A	486	CFZ	C2-N3	4.05	1.44	1.36
1	A	210	CFZ	C2-N3	4.05	1.44	1.36
1	A	335	CFZ	C2-N3	4.05	1.44	1.36
1	A	585	CFZ	C2-N3	4.05	1.44	1.36
1	A	247	CFZ	C2-N3	4.05	1.44	1.36
1	B	96	CFZ	C2-N3	4.05	1.44	1.36
1	A	149	CFZ	C2-N3	4.05	1.44	1.36
1	A	353	CFZ	C2-N3	4.05	1.44	1.36
1	B	587	CFZ	C2-N3	4.05	1.44	1.36
1	B	241	CFZ	C2-N3	4.05	1.44	1.36
1	B	604	CFZ	C2-N3	4.05	1.44	1.36
1	B	614	CFZ	C2-N3	4.05	1.44	1.36
1	A	631	CFZ	C2-N3	4.05	1.44	1.36
1	A	26	CFZ	C2-N3	4.05	1.44	1.36
1	B	120	CFZ	C2-N3	4.05	1.44	1.36
1	B	512	CFZ	C2-N3	4.05	1.44	1.36
1	A	523	CFZ	C2-N3	4.05	1.44	1.36
1	A	528	CFZ	C2-N3	4.05	1.44	1.36
1	B	585	CFZ	C2-N3	4.05	1.44	1.36
1	B	535	UFT	C2'-C3'	-4.04	1.47	1.52
1	A	246	CFZ	C2-N3	4.04	1.44	1.36
1	B	632	CFZ	C2-N3	4.04	1.44	1.36
1	A	285	CFZ	C2-N3	4.04	1.44	1.36
1	A	360	CFZ	C2-N3	4.04	1.44	1.36
1	A	362	CFZ	C2-N3	4.04	1.44	1.36
1	B	637	CFZ	C2-N3	4.04	1.44	1.36
1	A	153	UFT	C2'-C3'	-4.04	1.47	1.52
1	B	325	CFZ	C2-N3	4.04	1.44	1.36
1	A	477	CFZ	C2-N3	4.04	1.44	1.36
1	A	592	CFZ	C2-N3	4.04	1.44	1.36
1	A	110	CFZ	C2-N3	4.04	1.44	1.36
1	A	359	UFT	C2'-C3'	-4.04	1.47	1.52
1	A	34	CFZ	C2-N3	4.04	1.44	1.36
1	B	664	CFZ	C2-N3	4.04	1.44	1.36
1	A	21	CFZ	C2-N3	4.04	1.44	1.36
1	A	140	CFZ	C2-N3	4.04	1.44	1.36
1	A	425	CFZ	C2-N3	4.04	1.44	1.36
1	A	439	CFZ	C2-N3	4.04	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	506	CFZ	C2-N3	4.04	1.44	1.36
1	B	131	CFZ	C2-N3	4.04	1.44	1.36
1	A	19	UFT	C2'-C3'	-4.04	1.47	1.52
1	A	80	UFT	C2'-C3'	-4.04	1.47	1.52
1	B	406	CFZ	C2-N3	4.04	1.44	1.36
1	B	80	UFT	C2'-C3'	-4.04	1.47	1.52
1	B	389	UFT	C2'-C3'	-4.04	1.47	1.52
1	B	49	CFZ	C2-N3	4.04	1.44	1.36
1	B	548	CFZ	C2-N3	4.04	1.44	1.36
1	B	164	CFZ	C2-N3	4.04	1.44	1.36
1	B	458	CFZ	C2-N3	4.04	1.44	1.36
1	B	610	CFZ	C2-N3	4.04	1.44	1.36
1	A	614	CFZ	C2-N3	4.04	1.44	1.36
1	A	643	CFZ	C2-N3	4.04	1.44	1.36
1	B	209	CFZ	C2-N3	4.04	1.44	1.36
1	B	354	CFZ	C2-N3	4.04	1.44	1.36
1	B	579	CFZ	C2-N3	4.04	1.44	1.36
1	A	164	CFZ	C2-N3	4.04	1.44	1.36
1	A	600	CFZ	C2-N3	4.04	1.44	1.36
1	B	700	CFZ	C2-N3	4.04	1.44	1.36
1	A	39	CFZ	C2-N3	4.04	1.44	1.36
1	B	440	CFZ	C2-N3	4.04	1.44	1.36
1	B	528	CFZ	C2-N3	4.04	1.44	1.36
1	B	556	CFZ	C2-N3	4.04	1.44	1.36
1	B	302	UFT	C5-C4	4.04	1.52	1.43
1	A	249	CFZ	C2-N3	4.04	1.44	1.36
1	B	438	CFZ	C2-N3	4.04	1.44	1.36
1	A	652	CFZ	C2-N3	4.04	1.44	1.36
1	A	664	CFZ	C2-N3	4.04	1.44	1.36
1	B	171	CFZ	C2-N3	4.04	1.44	1.36
1	B	210	CFZ	C2-N3	4.04	1.44	1.36
1	A	383	CFZ	C2-N3	4.04	1.44	1.36
1	B	720	UFT	C2'-C3'	-4.04	1.47	1.52
1	A	188	CFZ	C2-N3	4.04	1.44	1.36
1	B	328	CFZ	C2-N3	4.04	1.44	1.36
1	A	370	CFZ	C2-N3	4.04	1.44	1.36
1	A	469	CFZ	C2-N3	4.04	1.44	1.36
1	A	421	UFT	C2'-C3'	-4.04	1.47	1.52
1	B	432	UFT	C2'-C3'	-4.04	1.47	1.52
1	A	46	CFZ	C2-N3	4.04	1.44	1.36
1	A	157	CFZ	C2-N3	4.04	1.44	1.36
1	B	492	CFZ	C2-N3	4.04	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	536	CFZ	C2-N3	4.04	1.44	1.36
1	B	104	CFZ	C2-N3	4.03	1.44	1.36
1	A	349	CFZ	C2-N3	4.03	1.44	1.36
1	B	351	CFZ	C2-N3	4.03	1.44	1.36
1	A	424	CFZ	C2-N3	4.03	1.44	1.36
1	B	625	CFZ	C2-N3	4.03	1.44	1.36
1	B	639	CFZ	C2-N3	4.03	1.44	1.36
1	B	456	UFT	C2'-C3'	-4.03	1.47	1.52
1	B	499	UFT	C2'-C3'	-4.03	1.47	1.52
1	B	151	CFZ	C2-N3	4.03	1.44	1.36
1	B	381	CFZ	C2-N3	4.03	1.44	1.36
1	A	75	CFZ	C2-N3	4.03	1.44	1.36
1	B	90	CFZ	C2-N3	4.03	1.44	1.36
1	B	407	CFZ	C2-N3	4.03	1.44	1.36
1	A	441	CFZ	C2-N3	4.03	1.44	1.36
1	A	704	CFZ	C2-N3	4.03	1.44	1.36
1	A	215	UFT	C5-C4	4.03	1.52	1.43
1	B	201	CFZ	C2-N3	4.03	1.44	1.36
1	B	229	UFT	C2'-C3'	-4.03	1.47	1.52
1	A	268	CFZ	C2-N3	4.03	1.44	1.36
1	B	424	CFZ	C2-N3	4.03	1.44	1.36
1	A	90	CFZ	C2-N3	4.03	1.44	1.36
1	A	198	CFZ	C2-N3	4.03	1.44	1.36
1	B	157	CFZ	C2-N3	4.03	1.44	1.36
1	A	104	CFZ	C2-N3	4.03	1.44	1.36
1	A	418	CFZ	C2-N3	4.03	1.44	1.36
1	B	418	CFZ	C2-N3	4.03	1.44	1.36
1	A	462	CFZ	C2-N3	4.03	1.44	1.36
1	B	477	CFZ	C2-N3	4.03	1.44	1.36
1	A	583	CFZ	C2-N3	4.03	1.44	1.36
1	B	73	CFZ	C2-N3	4.03	1.44	1.36
1	A	79	CFZ	C2-N3	4.03	1.44	1.36
1	B	234	CFZ	C2-N3	4.03	1.44	1.36
1	A	363	CFZ	C2-N3	4.03	1.44	1.36
1	A	620	CFZ	C2-N3	4.03	1.44	1.36
1	B	26	CFZ	C2-N3	4.03	1.44	1.36
1	A	682	CFZ	C2-N3	4.03	1.44	1.36
1	A	389	UFT	C2'-C3'	-4.03	1.47	1.52
1	A	676	UFT	C2'-C3'	-4.03	1.47	1.52
1	B	232	CFZ	C2-N3	4.03	1.44	1.36
1	A	25	CFZ	C2-N3	4.03	1.44	1.36
1	B	387	CFZ	C2-N3	4.03	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	651	CFZ	C2-N3	4.03	1.44	1.36
1	B	659	UFT	C2'-C3'	-4.03	1.47	1.52
1	B	247	CFZ	C2-N3	4.03	1.44	1.36
1	A	76	CFZ	C2-N3	4.03	1.44	1.36
1	B	353	CFZ	C2-N3	4.03	1.44	1.36
1	A	691	CFZ	C2-N3	4.03	1.44	1.36
1	B	198	CFZ	C2-N3	4.03	1.44	1.36
1	A	332	CFZ	C2-N3	4.03	1.44	1.36
1	B	574	CFZ	C2-N3	4.03	1.44	1.36
1	A	404	CFZ	C2-N3	4.02	1.44	1.36
1	B	404	CFZ	C2-N3	4.02	1.44	1.36
1	A	322	UFT	C2'-C3'	-4.02	1.47	1.52
1	B	21	CFZ	C2-N3	4.02	1.44	1.36
1	A	63	CFZ	C2-N3	4.02	1.44	1.36
1	A	381	CFZ	C2-N3	4.02	1.44	1.36
1	A	473	CFZ	C2-N3	4.02	1.44	1.36
1	A	693	CFZ	C2-N3	4.02	1.44	1.36
1	B	156	CFZ	C2-N3	4.02	1.44	1.36
1	A	351	CFZ	C2-N3	4.02	1.44	1.36
1	A	633	UFT	C2'-C3'	-4.02	1.47	1.52
1	B	10	CFZ	C2-N3	4.02	1.44	1.36
1	B	144	CFZ	C2-N3	4.02	1.44	1.36
1	B	384	CFZ	C2-N3	4.02	1.44	1.36
1	B	417	CFZ	C2-N3	4.02	1.44	1.36
1	A	407	CFZ	C2-N3	4.02	1.44	1.36
1	B	620	CFZ	C2-N3	4.02	1.44	1.36
1	B	208	UFT	C2'-C3'	-4.02	1.47	1.52
1	A	432	UFT	C2'-C3'	-4.02	1.47	1.52
1	A	703	UFT	C2'-C3'	-4.02	1.47	1.52
1	A	399	CFZ	C2-N3	4.02	1.44	1.36
1	B	67	CFZ	C2-N3	4.02	1.44	1.36
1	B	130	CFZ	C2-N3	4.02	1.44	1.36
1	A	494	CFZ	C2-N3	4.02	1.44	1.36
1	A	234	CFZ	C2-N3	4.02	1.44	1.36
1	B	691	CFZ	C2-N3	4.02	1.44	1.36
1	A	135	UFT	C2'-C3'	-4.02	1.47	1.52
1	B	367	UFT	C2'-C3'	-4.02	1.47	1.52
1	B	523	CFZ	C2-N3	4.02	1.44	1.36
1	B	188	CFZ	C2-N3	4.02	1.44	1.36
1	A	536	CFZ	C2-N3	4.02	1.44	1.36
1	B	405	CFZ	C2-N3	4.02	1.44	1.36
1	A	579	CFZ	C2-N3	4.02	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	CFZ	C2-N3	4.02	1.44	1.36
1	B	369	CFZ	C2-N3	4.02	1.44	1.36
1	A	543	CFZ	C2-N3	4.02	1.44	1.36
1	A	282	CFZ	C2-N3	4.01	1.44	1.36
1	A	219	CFZ	C2-N3	4.01	1.44	1.36
1	A	411	CFZ	C2-N3	4.01	1.44	1.36
1	A	451	CFZ	C2-N3	4.01	1.44	1.36
1	B	332	CFZ	C2-N3	4.01	1.44	1.36
1	B	473	CFZ	C2-N3	4.01	1.44	1.36
1	A	130	CFZ	C2-N3	4.01	1.44	1.36
1	A	212	CFZ	C2-N3	4.01	1.44	1.36
1	B	33	UFT	C2'-C3'	-4.01	1.47	1.52
1	A	72	CFZ	C2-N3	4.01	1.44	1.36
1	B	46	CFZ	C2-N3	4.01	1.44	1.36
1	A	44	UFT	C2'-C3'	-4.01	1.47	1.52
1	A	251	UFT	C2'-C3'	-4.01	1.47	1.52
1	A	384	CFZ	C2-N3	4.01	1.44	1.36
1	A	700	CFZ	C2-N3	4.01	1.44	1.36
1	B	360	CFZ	C2-N3	4.01	1.44	1.36
1	B	117	CFZ	C2-N3	4.01	1.44	1.36
1	B	140	CFZ	C2-N3	4.01	1.44	1.36
1	A	378	CFZ	C2-N3	4.01	1.44	1.36
1	A	556	CFZ	C2-N3	4.01	1.44	1.36
1	B	135	UFT	C2'-C3'	-4.01	1.47	1.52
1	B	363	CFZ	C2-N3	4.01	1.44	1.36
1	A	657	CFZ	C2-N3	4.01	1.44	1.36
1	B	111	CFZ	C2-N3	4.00	1.44	1.36
1	A	129	CFZ	C2-N3	4.00	1.44	1.36
1	B	378	CFZ	C2-N3	4.00	1.44	1.36
1	B	283	UFT	C2'-C3'	-4.00	1.47	1.52
1	B	28	CFZ	C2-N3	4.00	1.44	1.36
1	A	216	UFT	C5-C4	4.00	1.52	1.43
1	A	216	UFT	C2'-C3'	-4.00	1.47	1.52
1	B	646	UFT	C2'-C3'	-4.00	1.47	1.52
1	A	111	CFZ	C2-N3	4.00	1.44	1.36
1	A	293	UFT	C2'-C3'	-4.00	1.47	1.52
1	B	34	CFZ	C2-N3	4.00	1.44	1.36
1	B	153	UFT	C2'-C3'	-4.00	1.47	1.52
1	A	217	UFT	C2'-C3'	-4.00	1.47	1.52
1	B	421	UFT	C2'-C3'	-4.00	1.47	1.52
1	A	354	CFZ	C2-N3	4.00	1.44	1.36
1	B	165	CFZ	C2-N3	3.99	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	CFZ	C2-N3	3.99	1.44	1.36
1	B	32	UFT	C2'-C3'	-3.99	1.47	1.52
1	A	576	CFZ	C2-N3	3.99	1.44	1.36
1	B	184	CFZ	C2-N3	3.99	1.44	1.36
1	A	464	UFT	C2'-C3'	-3.99	1.47	1.52
1	B	524	UFT	C2'-C3'	-3.99	1.47	1.52
1	B	633	UFT	C2'-C3'	-3.99	1.47	1.52
1	A	165	CFZ	C2-N3	3.99	1.44	1.36
1	B	293	UFT	C2'-C3'	-3.99	1.47	1.52
1	A	602	UFT	C2'-C3'	-3.99	1.47	1.52
1	B	708	UFT	C2'-C3'	-3.99	1.47	1.52
1	B	8	UFT	C2'-C3'	-3.99	1.47	1.52
1	B	44	UFT	C2'-C3'	-3.99	1.47	1.52
1	B	518	CFZ	C2'-C3'	-3.99	1.47	1.52
1	B	565	CFZ	C2-N3	3.98	1.44	1.36
1	B	129	CFZ	C2-N3	3.98	1.44	1.36
1	B	643	CFZ	C2-N3	3.98	1.44	1.36
1	A	551	CFZ	C2-N3	3.98	1.44	1.36
1	A	518	CFZ	C2-N3	3.98	1.44	1.36
1	B	15	CFZ	C2-N3	3.98	1.44	1.36
1	B	92	UFT	C2'-C3'	-3.98	1.47	1.52
1	A	592	CFZ	C2'-C3'	-3.98	1.47	1.52
1	A	50	UFT	C2'-C3'	-3.98	1.47	1.52
1	B	489	UFT	C2'-C3'	-3.98	1.47	1.52
1	A	97	UFT	C2'-C3'	-3.98	1.47	1.52
1	A	208	UFT	C2'-C3'	-3.98	1.47	1.52
1	B	545	UFT	C2'-C3'	-3.98	1.47	1.52
1	A	329	UFT	C2'-C3'	-3.98	1.47	1.52
1	A	302	UFT	C2'-C3'	-3.97	1.47	1.52
1	A	350	UFT	C2'-C3'	-3.97	1.47	1.52
1	B	365	UFT	C2'-C3'	-3.97	1.47	1.52
1	A	499	UFT	C2'-C3'	-3.97	1.47	1.52
1	B	543	CFZ	C2-N3	3.97	1.44	1.36
1	B	676	UFT	C2'-C3'	-3.97	1.47	1.52
1	A	49	CFZ	C2-N3	3.97	1.44	1.36
1	A	387	CFZ	C2-N3	3.97	1.44	1.36
1	B	26	CFZ	C2'-C3'	-3.97	1.47	1.52
1	B	19	UFT	C2'-C3'	-3.97	1.47	1.52
1	A	215	UFT	C2'-C3'	-3.97	1.47	1.52
1	A	659	UFT	C2'-C3'	-3.97	1.47	1.52
1	A	402	UFT	C2'-C3'	-3.97	1.47	1.52
1	B	217	UFT	C2'-C3'	-3.96	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	456	UFT	C2'-C3'	-3.96	1.47	1.52
1	B	695	UFT	C2'-C3'	-3.96	1.47	1.52
1	A	712	UFT	C2'-C3'	-3.96	1.47	1.52
1	B	602	UFT	C2'-C3'	-3.96	1.47	1.52
1	A	179	UFT	C2'-C3'	-3.96	1.47	1.52
1	B	75	CFZ	C2-N3	3.96	1.44	1.36
1	A	92	UFT	C2'-C3'	-3.96	1.47	1.52
1	A	175	UFT	C2'-C3'	-3.96	1.47	1.52
1	B	352	UFT	C2'-C3'	-3.96	1.47	1.52
1	B	423	UFT	C2'-C3'	-3.96	1.47	1.52
1	B	97	UFT	C2'-C3'	-3.96	1.47	1.52
1	A	646	UFT	C2'-C3'	-3.96	1.47	1.52
1	B	313	UFT	C2'-C3'	-3.95	1.47	1.52
1	B	712	UFT	C2'-C3'	-3.95	1.47	1.52
1	B	491	CFZ	C2-N3	3.95	1.44	1.36
1	B	302	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	708	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	14	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	447	UFT	C2'-C3'	-3.94	1.47	1.52
1	B	464	UFT	C2'-C3'	-3.94	1.47	1.52
1	A	11	UFT	C2'-C3'	-3.94	1.47	1.52
1	B	534	UFT	C2'-C3'	-3.94	1.47	1.52
1	A	265	UFT	C2'-C3'	-3.94	1.47	1.52
1	B	359	UFT	C2'-C3'	-3.94	1.47	1.52
1	A	471	UFT	C2'-C3'	-3.94	1.47	1.52
1	A	204	UFT	C2'-C3'	-3.94	1.47	1.52
1	B	321	CFZ	C2-N3	3.94	1.44	1.36
1	B	549	UFT	C2'-C3'	-3.94	1.47	1.52
1	A	695	UFT	C2'-C3'	-3.93	1.47	1.52
1	B	493	UFT	C5-C4	3.93	1.52	1.43
1	B	669	UFT	C2'-C3'	-3.93	1.47	1.52
1	B	344	UFT	C2'-C3'	-3.93	1.47	1.52
1	B	192	UFT	C2'-C3'	-3.93	1.47	1.52
1	B	204	UFT	C2'-C3'	-3.93	1.47	1.52
1	A	362	CFZ	C2'-C3'	-3.93	1.47	1.52
1	A	534	UFT	C2'-C3'	-3.93	1.47	1.52
1	B	163	UFT	C2'-C3'	-3.93	1.47	1.52
1	B	322	UFT	C2'-C3'	-3.93	1.47	1.52
1	B	629	UFT	C2'-C3'	-3.93	1.47	1.52
1	A	309	UFT	C2'-C3'	-3.92	1.47	1.52
1	A	377	UFT	C2'-C3'	-3.92	1.47	1.52
1	B	402	UFT	C2'-C3'	-3.92	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	509	UFT	C2'-C3'	-3.92	1.47	1.52
1	A	59	UFT	C2'-C3'	-3.91	1.47	1.52
1	A	423	UFT	C2'-C3'	-3.91	1.47	1.52
1	A	545	UFT	C2'-C3'	-3.91	1.47	1.52
1	A	542	UFT	C2'-C3'	-3.91	1.47	1.52
1	B	571	UFT	C2'-C3'	-3.91	1.47	1.52
1	B	471	UFT	C2'-C3'	-3.91	1.47	1.52
1	A	577	UFT	C2'-C3'	-3.91	1.47	1.52
1	A	629	UFT	C2'-C3'	-3.91	1.47	1.52
1	A	229	UFT	C2'-C3'	-3.91	1.47	1.52
1	A	571	UFT	C2'-C3'	-3.91	1.47	1.52
1	B	481	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	481	UFT	C2'-C3'	-3.90	1.47	1.52
1	B	542	UFT	C2'-C3'	-3.90	1.47	1.52
1	B	214	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	669	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	98	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	163	UFT	C2'-C3'	-3.90	1.47	1.52
1	B	447	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	549	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	137	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	192	UFT	C2'-C3'	-3.90	1.47	1.52
1	B	460	UFT	C2'-C3'	-3.90	1.47	1.52
1	B	577	UFT	C2'-C3'	-3.90	1.47	1.52
1	B	690	UFT	C2'-C3'	-3.89	1.47	1.52
1	A	653	UFT	C2'-C3'	-3.89	1.47	1.52
1	A	8	UFT	C2'-C3'	-3.89	1.47	1.52
1	B	55	UFT	C2'-C3'	-3.89	1.47	1.52
1	B	398	UFT	C2'-C3'	-3.89	1.47	1.52
1	A	94	UFT	C2'-C3'	-3.89	1.47	1.52
1	B	329	UFT	C2'-C3'	-3.89	1.47	1.52
1	A	687	UFT	C2'-C3'	-3.89	1.47	1.52
1	B	530	UFT	C2'-C3'	-3.89	1.47	1.52
1	A	690	UFT	C2'-C3'	-3.88	1.47	1.52
1	B	84	UFT	C2'-C3'	-3.88	1.47	1.52
1	B	86	UFT	C2'-C3'	-3.88	1.47	1.52
1	B	377	UFT	C2'-C3'	-3.88	1.47	1.52
1	B	14	UFT	C2'-C3'	-3.88	1.47	1.52
1	A	55	UFT	C2'-C3'	-3.88	1.47	1.52
1	B	112	UFT	C2'-C3'	-3.88	1.47	1.52
1	A	460	UFT	C2'-C3'	-3.88	1.47	1.52
1	A	112	UFT	C2'-C3'	-3.88	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	UFT	C2'-C3'	-3.88	1.47	1.52
1	A	398	UFT	C2'-C3'	-3.87	1.47	1.52
1	B	687	UFT	C2'-C3'	-3.87	1.47	1.52
1	B	590	UFT	C2'-C3'	-3.87	1.47	1.52
1	A	607	UFT	C2'-C3'	-3.87	1.47	1.52
1	B	175	UFT	C2'-C3'	-3.87	1.47	1.52
1	B	509	UFT	C2'-C3'	-3.87	1.47	1.52
1	B	98	UFT	C2'-C3'	-3.87	1.47	1.52
1	B	11	UFT	C2'-C3'	-3.87	1.47	1.52
1	B	265	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	266	UFT	C2'-C3'	-3.86	1.47	1.52
1	B	431	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	141	UFT	C2'-C3'	-3.86	1.47	1.52
1	B	559	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	84	UFT	C2'-C3'	-3.85	1.47	1.52
1	B	137	UFT	C2'-C3'	-3.85	1.47	1.52
1	B	334	UFT	C2'-C3'	-3.85	1.47	1.52
1	B	141	UFT	C2'-C3'	-3.84	1.47	1.52
1	A	635	UFT	C2'-C3'	-3.84	1.47	1.52
1	A	581	UFT	C2'-C3'	-3.83	1.47	1.52
1	A	86	UFT	C2'-C3'	-3.83	1.47	1.52
1	A	689	UFT	C2'-C3'	-3.83	1.47	1.52
1	B	71	UFT	C2'-C3'	-3.83	1.47	1.52
1	A	174	UFT	C2'-C3'	-3.83	1.47	1.52
1	B	689	UFT	C2'-C3'	-3.83	1.47	1.52
1	A	431	UFT	C2'-C3'	-3.82	1.47	1.52
1	B	94	UFT	C2'-C3'	-3.82	1.47	1.52
1	B	106	UFT	C2'-C3'	-3.82	1.47	1.52
1	B	266	UFT	C2'-C3'	-3.82	1.47	1.52
1	A	155	UFT	C2'-C3'	-3.82	1.47	1.52
1	B	519	UFT	C2'-C3'	-3.82	1.47	1.52
1	B	59	UFT	C2'-C3'	-3.81	1.47	1.52
1	A	485	UFT	C2'-C3'	-3.81	1.47	1.52
1	B	61	UFT	C2'-C3'	-3.81	1.47	1.52
1	A	197	UFT	C2'-C3'	-3.81	1.47	1.52
1	B	504	UFT	C2'-C3'	-3.81	1.47	1.52
1	B	653	UFT	C2'-C3'	-3.81	1.47	1.52
1	B	233	UFT	C2'-C3'	-3.81	1.47	1.52
1	B	154	UFT	C2'-C3'	-3.81	1.47	1.52
1	B	48	UFT	C2'-C3'	-3.81	1.47	1.52
1	B	485	UFT	C2'-C3'	-3.81	1.47	1.52
1	B	701	UFT	C2'-C3'	-3.80	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	UFT	C2'-C3'	-3.80	1.47	1.52
1	A	701	UFT	C2'-C3'	-3.80	1.47	1.52
1	B	190	UFT	C2'-C3'	-3.80	1.47	1.52
1	A	559	UFT	C2'-C3'	-3.80	1.47	1.52
1	A	106	UFT	C2'-C3'	-3.80	1.47	1.52
1	A	32	UFT	C2'-C3'	-3.80	1.47	1.52
1	B	554	UFT	C2'-C3'	-3.80	1.47	1.52
1	B	169	UFT	C2'-C3'	-3.80	1.47	1.52
1	A	142	UFT	C2'-C3'	-3.80	1.47	1.52
1	A	245	UFT	C2'-C3'	-3.80	1.47	1.52
1	B	88	UFT	C2'-C3'	-3.80	1.47	1.52
1	A	115	UFT	C2'-C3'	-3.80	1.47	1.52
1	A	334	UFT	C2'-C3'	-3.80	1.47	1.52
1	A	154	UFT	C2'-C3'	-3.79	1.47	1.52
1	A	403	UFT	C2'-C3'	-3.79	1.47	1.52
1	B	309	UFT	C2'-C3'	-3.79	1.47	1.52
1	B	336	UFT	C2'-C3'	-3.79	1.47	1.52
1	A	160	UFT	C2'-C3'	-3.79	1.47	1.52
1	B	174	UFT	C2'-C3'	-3.79	1.47	1.52
1	A	504	UFT	C2'-C3'	-3.79	1.47	1.52
1	B	635	UFT	C2'-C3'	-3.79	1.47	1.52
1	A	202	UFT	C2'-C3'	-3.79	1.47	1.52
1	A	720	UFT	C2'-C3'	-3.79	1.47	1.52
1	A	618	UFT	C2'-C3'	-3.78	1.47	1.52
1	A	666	UFT	C2'-C3'	-3.78	1.47	1.52
1	B	696	UFT	C2'-C3'	-3.78	1.47	1.52
1	B	142	UFT	C2'-C3'	-3.78	1.47	1.52
1	A	89	UFT	C2'-C3'	-3.78	1.47	1.52
1	B	296	UFT	C2'-C3'	-3.78	1.47	1.52
1	B	155	UFT	C2'-C3'	-3.78	1.47	1.52
1	B	719	UFT	C2'-C3'	-3.78	1.47	1.52
1	A	61	UFT	C2'-C3'	-3.78	1.47	1.52
1	A	88	UFT	C2'-C3'	-3.77	1.47	1.52
1	A	673	UFT	C2'-C3'	-3.77	1.47	1.52
1	A	696	UFT	C2'-C3'	-3.77	1.47	1.52
1	A	347	UFT	C2'-C3'	-3.77	1.47	1.52
1	A	296	UFT	C2'-C3'	-3.77	1.47	1.52
1	B	666	UFT	C2'-C3'	-3.77	1.47	1.52
1	B	197	UFT	C2'-C3'	-3.77	1.47	1.52
1	B	434	UFT	C2'-C3'	-3.77	1.47	1.52
1	A	430	UFT	C2'-C3'	-3.77	1.47	1.52
1	B	662	UFT	C2'-C3'	-3.77	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	581	UFT	C2'-C3'	-3.77	1.47	1.52
1	A	628	UFT	C2'-C3'	-3.76	1.47	1.52
1	B	202	UFT	C2'-C3'	-3.76	1.47	1.52
1	B	115	UFT	C2'-C3'	-3.76	1.47	1.52
1	A	636	UFT	C2'-C3'	-3.76	1.47	1.52
1	A	503	UFT	C2'-C3'	-3.76	1.47	1.52
1	A	48	UFT	C2'-C3'	-3.76	1.47	1.52
1	A	662	UFT	C2'-C3'	-3.76	1.47	1.52
1	B	403	UFT	C2'-C3'	-3.75	1.47	1.52
1	A	344	UFT	C2'-C3'	-3.75	1.47	1.52
1	A	170	UFT	C2'-C3'	-3.75	1.47	1.52
1	B	607	UFT	C2'-C3'	-3.75	1.47	1.52
1	B	592	CFZ	C2'-C3'	-3.75	1.47	1.52
1	B	366	UFT	C2'-C3'	-3.75	1.47	1.52
1	A	196	UFT	C2'-C3'	-3.75	1.47	1.52
1	B	62	UFT	C2'-C3'	-3.74	1.47	1.52
1	B	196	UFT	C2'-C3'	-3.74	1.47	1.52
1	B	89	UFT	C2'-C3'	-3.74	1.47	1.52
1	A	554	UFT	C2'-C3'	-3.74	1.47	1.52
1	A	500	UFT	C2'-C3'	-3.74	1.47	1.52
1	B	673	UFT	C2'-C3'	-3.74	1.47	1.52
1	B	347	UFT	C2'-C3'	-3.74	1.47	1.52
1	A	593	UFT	C2'-C3'	-3.74	1.47	1.52
1	B	608	UFT	C2'-C3'	-3.74	1.47	1.52
1	A	609	UFT	C2'-C3'	-3.74	1.47	1.52
1	A	190	UFT	C2'-C3'	-3.74	1.47	1.52
1	B	160	UFT	C2'-C3'	-3.74	1.47	1.52
1	B	215	UFT	C2'-C3'	-3.74	1.47	1.52
1	A	656	UFT	C2'-C3'	-3.74	1.47	1.52
1	B	618	UFT	C2'-C3'	-3.73	1.47	1.52
1	A	143	UFT	C2'-C3'	-3.73	1.47	1.52
1	A	126	UFT	C2'-C3'	-3.73	1.47	1.52
1	A	361	UFT	C2'-C3'	-3.73	1.47	1.52
1	A	472	UFT	C2'-C3'	-3.73	1.47	1.52
1	B	656	UFT	C2'-C3'	-3.73	1.47	1.52
1	A	74	UFT	C2'-C3'	-3.73	1.47	1.52
1	B	628	UFT	C2'-C3'	-3.73	1.47	1.52
1	A	366	UFT	C2'-C3'	-3.72	1.47	1.52
1	A	116	UFT	C2'-C3'	-3.72	1.47	1.52
1	B	69	UFT	C2'-C3'	-3.72	1.47	1.52
1	B	101	UFT	C2'-C3'	-3.72	1.47	1.52
1	A	434	UFT	C2'-C3'	-3.72	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	170	UFT	C2'-C3'	-3.71	1.47	1.52
1	B	609	UFT	C2'-C3'	-3.71	1.47	1.52
1	A	39	CFZ	O2-C2	3.71	1.30	1.23
1	A	71	UFT	C2'-C3'	-3.71	1.47	1.52
1	B	126	UFT	C2'-C3'	-3.71	1.47	1.52
1	A	336	UFT	C2'-C3'	-3.71	1.47	1.52
1	B	120	CFZ	O2-C2	3.70	1.30	1.23
1	A	354	CFZ	C2'-C3'	-3.70	1.47	1.52
1	A	489	UFT	C2'-C3'	-3.70	1.47	1.52
1	A	424	CFZ	O2-C2	3.70	1.30	1.23
1	B	143	UFT	C2'-C3'	-3.70	1.47	1.52
1	A	69	UFT	C2'-C3'	-3.70	1.47	1.52
1	A	355	CFZ	C2'-C3'	-3.70	1.47	1.52
1	A	43	UFT	C2'-C3'	-3.69	1.47	1.52
1	B	430	UFT	C2'-C3'	-3.69	1.47	1.52
1	A	466	UFT	C2'-C3'	-3.69	1.47	1.52
1	A	590	UFT	C2'-C3'	-3.69	1.47	1.52
1	A	608	UFT	C2'-C3'	-3.69	1.47	1.52
1	B	46	CFZ	O2-C2	3.69	1.30	1.23
1	B	502	UFT	C2'-C3'	-3.69	1.47	1.52
1	B	424	CFZ	O2-C2	3.69	1.30	1.23
1	B	116	UFT	C2'-C3'	-3.69	1.47	1.52
1	B	441	CFZ	O2-C2	3.69	1.30	1.23
1	B	270	UFT	C2'-C3'	-3.69	1.47	1.52
1	B	43	UFT	C2'-C3'	-3.69	1.47	1.52
1	B	636	UFT	C2'-C3'	-3.68	1.47	1.52
1	A	352	UFT	C2'-C3'	-3.68	1.47	1.52
1	B	555	UFT	C2'-C3'	-3.68	1.47	1.52
1	B	13	UFT	C2'-C3'	-3.68	1.47	1.52
1	A	555	UFT	C2'-C3'	-3.68	1.47	1.52
1	B	39	CFZ	O2-C2	3.68	1.30	1.23
1	B	500	UFT	C2'-C3'	-3.68	1.47	1.52
1	A	301	UFT	C2'-C3'	-3.68	1.47	1.52
1	B	50	UFT	C2'-C3'	-3.68	1.47	1.52
1	B	34	CFZ	O2-C2	3.67	1.30	1.23
1	A	10	CFZ	O2-C2	3.67	1.30	1.23
1	A	62	UFT	C2'-C3'	-3.67	1.47	1.52
1	A	120	CFZ	O2-C2	3.67	1.30	1.23
1	A	719	UFT	C2'-C3'	-3.67	1.47	1.52
1	A	387	CFZ	O2-C2	3.67	1.30	1.23
1	A	502	UFT	C2'-C3'	-3.66	1.47	1.52
1	B	49	CFZ	O2-C2	3.66	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	CFZ	O2-C2	3.66	1.30	1.23
1	A	233	UFT	C2'-C3'	-3.66	1.47	1.52
1	B	466	UFT	C2'-C3'	-3.66	1.47	1.52
1	B	540	CFZ	O2-C2	3.66	1.30	1.23
1	B	156	CFZ	O2-C2	3.66	1.30	1.23
1	A	493	UFT	C2'-C3'	-3.66	1.47	1.52
1	A	540	CFZ	O2-C2	3.66	1.30	1.23
1	B	600	CFZ	O2-C2	3.66	1.30	1.23
1	A	156	CFZ	O2-C2	3.66	1.30	1.23
1	A	210	CFZ	O2-C2	3.66	1.30	1.23
1	A	600	CFZ	O2-C2	3.66	1.30	1.23
1	B	182	UFT	C2'-C3'	-3.66	1.47	1.52
1	B	472	UFT	C2'-C3'	-3.66	1.47	1.52
1	A	477	CFZ	O2-C2	3.66	1.30	1.23
1	B	663	UFT	C2'-C3'	-3.66	1.47	1.52
1	B	279	CFZ	O2-C2	3.65	1.30	1.23
1	A	370	CFZ	O2-C2	3.65	1.30	1.23
1	B	285	CFZ	O2-C2	3.65	1.30	1.23
1	B	298	CFZ	O2-C2	3.65	1.30	1.23
1	A	455	CFZ	O2-C2	3.65	1.30	1.23
1	A	517	CFZ	O2-C2	3.65	1.30	1.23
1	A	335	CFZ	O2-C2	3.65	1.30	1.23
1	B	498	CFZ	O2-C2	3.65	1.30	1.23
1	B	536	CFZ	O2-C2	3.65	1.30	1.23
1	B	565	CFZ	O2-C2	3.65	1.30	1.23
1	B	325	CFZ	O2-C2	3.65	1.30	1.23
1	A	79	CFZ	O2-C2	3.64	1.30	1.23
1	B	129	CFZ	O2-C2	3.64	1.30	1.23
1	A	353	CFZ	O2-C2	3.64	1.30	1.23
1	A	651	CFZ	O2-C2	3.64	1.30	1.23
1	A	129	CFZ	O2-C2	3.64	1.30	1.23
1	A	212	CFZ	O2-C2	3.64	1.30	1.23
1	A	406	CFZ	O2-C2	3.64	1.30	1.23
1	B	242	CFZ	O2-C2	3.64	1.30	1.23
1	A	383	CFZ	O2-C2	3.64	1.30	1.23
1	A	182	UFT	C2'-C3'	-3.64	1.47	1.52
1	B	198	CFZ	O2-C2	3.64	1.30	1.23
1	A	655	CFZ	O2-C2	3.64	1.30	1.23
1	A	21	CFZ	O2-C2	3.64	1.30	1.23
1	A	304	CFZ	O2-C2	3.64	1.30	1.23
1	B	528	CFZ	O2-C2	3.64	1.30	1.23
1	A	34	CFZ	O2-C2	3.64	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	568	CFZ	O2-C2	3.64	1.30	1.23
1	A	663	UFT	C2'-C3'	-3.64	1.47	1.52
1	A	104	CFZ	O2-C2	3.64	1.30	1.23
1	A	384	CFZ	O2-C2	3.64	1.30	1.23
1	B	698	CFZ	O2-C2	3.64	1.30	1.23
1	A	282	CFZ	O2-C2	3.64	1.30	1.23
1	B	387	CFZ	O2-C2	3.64	1.30	1.23
1	A	151	CFZ	O2-C2	3.64	1.30	1.23
1	A	219	CFZ	O2-C2	3.64	1.30	1.23
1	B	621	UFT	C2'-C3'	-3.64	1.47	1.52
1	B	381	CFZ	O2-C2	3.64	1.30	1.23
1	B	405	CFZ	O2-C2	3.63	1.30	1.23
1	B	241	CFZ	O2-C2	3.63	1.30	1.23
1	A	103	CFZ	O2-C2	3.63	1.30	1.23
1	A	565	CFZ	O2-C2	3.63	1.30	1.23
1	A	101	UFT	C2'-C3'	-3.63	1.47	1.52
1	A	544	UFT	C2'-C3'	-3.63	1.47	1.52
1	A	49	CFZ	O2-C2	3.63	1.30	1.23
1	A	325	CFZ	O2-C2	3.63	1.30	1.23
1	A	462	CFZ	O2-C2	3.63	1.30	1.23
1	A	704	CFZ	O2-C2	3.63	1.30	1.23
1	B	406	CFZ	O2-C2	3.63	1.30	1.23
1	A	523	CFZ	O2-C2	3.63	1.30	1.23
1	B	682	CFZ	O2-C2	3.63	1.30	1.23
1	B	209	CFZ	O2-C2	3.63	1.30	1.23
1	A	440	CFZ	O2-C2	3.63	1.30	1.23
1	A	625	CFZ	O2-C2	3.63	1.30	1.23
1	A	621	UFT	C2'-C3'	-3.63	1.47	1.52
1	A	130	CFZ	O2-C2	3.63	1.30	1.23
1	A	242	CFZ	O2-C2	3.63	1.30	1.23
1	A	518	CFZ	O2-C2	3.63	1.30	1.23
1	A	691	CFZ	O2-C2	3.63	1.30	1.23
1	B	614	CFZ	O2-C2	3.63	1.30	1.23
1	B	679	CFZ	O2-C2	3.63	1.30	1.23
1	B	338	CFZ	O2-C2	3.63	1.30	1.23
1	B	477	CFZ	O2-C2	3.63	1.30	1.23
1	B	144	CFZ	O2-C2	3.63	1.30	1.23
1	B	486	CFZ	O2-C2	3.63	1.30	1.23
1	A	494	CFZ	O2-C2	3.63	1.30	1.23
1	B	506	CFZ	O2-C2	3.63	1.30	1.23
1	A	603	CFZ	O2-C2	3.63	1.30	1.23
1	A	491	CFZ	O2-C2	3.63	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	301	UFT	C2'-C3'	-3.62	1.47	1.52
1	B	355	CFZ	O2-C2	3.62	1.30	1.23
1	B	369	CFZ	O2-C2	3.62	1.30	1.23
1	B	643	CFZ	O2-C2	3.62	1.30	1.23
1	B	140	CFZ	O2-C2	3.62	1.30	1.23
1	A	441	CFZ	O2-C2	3.62	1.30	1.23
1	B	74	UFT	C2'-C3'	-3.62	1.47	1.52
1	B	384	CFZ	O2-C2	3.62	1.30	1.23
1	B	568	CFZ	O2-C2	3.62	1.30	1.23
1	A	26	CFZ	O2-C2	3.62	1.30	1.23
1	B	232	CFZ	O2-C2	3.62	1.30	1.23
1	B	335	CFZ	O2-C2	3.62	1.30	1.23
1	A	551	CFZ	O2-C2	3.62	1.30	1.23
1	A	354	CFZ	O2-C2	3.62	1.30	1.23
1	A	474	CFZ	O2-C2	3.62	1.30	1.23
1	B	67	CFZ	O2-C2	3.62	1.30	1.23
1	A	206	CFZ	O2-C2	3.62	1.30	1.23
1	B	378	CFZ	O2-C2	3.62	1.30	1.23
1	A	382	CFZ	O2-C2	3.62	1.30	1.23
1	A	548	CFZ	O2-C2	3.62	1.30	1.23
1	A	620	CFZ	O2-C2	3.62	1.30	1.23
1	B	21	CFZ	O2-C2	3.62	1.30	1.23
1	A	63	CFZ	O2-C2	3.62	1.30	1.23
1	B	151	CFZ	O2-C2	3.62	1.30	1.23
1	B	164	CFZ	O2-C2	3.62	1.30	1.23
1	B	651	CFZ	O2-C2	3.62	1.30	1.23
1	A	46	CFZ	O2-C2	3.62	1.30	1.23
1	A	585	CFZ	O2-C2	3.62	1.30	1.23
1	A	270	UFT	C2'-C3'	-3.62	1.47	1.52
1	A	149	CFZ	O2-C2	3.62	1.30	1.23
1	B	149	CFZ	O2-C2	3.62	1.30	1.23
1	B	315	CFZ	O2-C2	3.62	1.30	1.23
1	A	381	CFZ	O2-C2	3.62	1.30	1.23
1	B	79	CFZ	O2-C2	3.62	1.30	1.23
1	B	188	CFZ	O2-C2	3.62	1.30	1.23
1	B	604	CFZ	O2-C2	3.62	1.30	1.23
1	B	103	CFZ	O2-C2	3.62	1.30	1.23
1	A	349	CFZ	O2-C2	3.62	1.30	1.23
1	A	411	CFZ	O2-C2	3.62	1.30	1.23
1	B	603	CFZ	O2-C2	3.62	1.30	1.23
1	B	130	CFZ	O2-C2	3.62	1.30	1.23
1	B	404	CFZ	O2-C2	3.62	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	CFZ	O2-C2	3.62	1.30	1.23
1	B	548	CFZ	O2-C2	3.62	1.30	1.23
1	B	574	CFZ	O2-C2	3.62	1.30	1.23
1	B	157	CFZ	O2-C2	3.61	1.30	1.23
1	B	90	CFZ	O2-C2	3.61	1.30	1.23
1	B	210	CFZ	O2-C2	3.61	1.30	1.23
1	A	418	CFZ	O2-C2	3.61	1.30	1.23
1	B	418	CFZ	O2-C2	3.61	1.30	1.23
1	A	558	CFZ	O2-C2	3.61	1.30	1.23
1	B	691	CFZ	O2-C2	3.61	1.30	1.23
1	A	188	CFZ	O2-C2	3.61	1.30	1.23
1	A	246	CFZ	O2-C2	3.61	1.30	1.23
1	A	249	CFZ	O2-C2	3.61	1.30	1.23
1	B	370	CFZ	O2-C2	3.61	1.30	1.23
1	A	439	CFZ	O2-C2	3.61	1.30	1.23
1	A	459	CFZ	O2-C2	3.61	1.30	1.23
1	A	631	CFZ	O2-C2	3.61	1.30	1.23
1	A	698	CFZ	O2-C2	3.61	1.30	1.23
1	A	700	CFZ	O2-C2	3.61	1.30	1.23
1	A	131	CFZ	O2-C2	3.61	1.30	1.23
1	B	363	CFZ	O2-C2	3.61	1.30	1.23
1	A	564	CFZ	O2-C2	3.61	1.30	1.23
1	B	308	CFZ	O2-C2	3.61	1.30	1.23
1	A	369	CFZ	O2-C2	3.61	1.30	1.23
1	A	556	CFZ	O2-C2	3.61	1.30	1.23
1	B	667	CFZ	O2-C2	3.61	1.30	1.23
1	A	28	CFZ	O2-C2	3.61	1.30	1.23
1	A	279	CFZ	O2-C2	3.61	1.30	1.23
1	A	355	CFZ	O2-C2	3.61	1.30	1.23
1	A	425	CFZ	O2-C2	3.61	1.30	1.23
1	A	652	CFZ	O2-C2	3.61	1.30	1.23
1	B	700	CFZ	O2-C2	3.61	1.30	1.23
1	B	10	CFZ	O2-C2	3.61	1.30	1.23
1	B	28	CFZ	O2-C2	3.61	1.30	1.23
1	A	110	CFZ	O2-C2	3.61	1.30	1.23
1	A	241	CFZ	O2-C2	3.61	1.30	1.23
1	B	438	CFZ	O2-C2	3.61	1.30	1.23
1	B	550	CFZ	O2-C2	3.61	1.30	1.23
1	A	579	CFZ	O2-C2	3.61	1.30	1.23
1	A	592	CFZ	O2-C2	3.61	1.30	1.23
1	A	610	CFZ	O2-C2	3.61	1.30	1.23
1	B	652	CFZ	O2-C2	3.61	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	CFZ	O2-C2	3.61	1.30	1.23
1	B	234	CFZ	O2-C2	3.61	1.30	1.23
1	A	247	CFZ	O2-C2	3.61	1.30	1.23
1	A	338	CFZ	O2-C2	3.61	1.30	1.23
1	A	436	CFZ	O2-C2	3.61	1.30	1.23
1	B	512	CFZ	O2-C2	3.61	1.30	1.23
1	B	543	CFZ	O2-C2	3.61	1.30	1.23
1	B	620	CFZ	O2-C2	3.61	1.30	1.23
1	B	184	CFZ	O2-C2	3.61	1.30	1.23
1	B	558	CFZ	O2-C2	3.61	1.30	1.23
1	B	212	CFZ	O2-C2	3.61	1.30	1.23
1	B	426	CFZ	O2-C2	3.61	1.30	1.23
1	B	458	CFZ	O2-C2	3.61	1.30	1.23
1	B	523	CFZ	O2-C2	3.61	1.30	1.23
1	A	67	CFZ	O2-C2	3.61	1.30	1.23
1	A	285	CFZ	O2-C2	3.61	1.30	1.23
1	B	362	CFZ	O2-C2	3.61	1.30	1.23
1	B	417	CFZ	O2-C2	3.61	1.30	1.23
1	A	90	CFZ	O2-C2	3.61	1.30	1.23
1	A	465	CFZ	O2-C2	3.61	1.30	1.23
1	B	579	CFZ	O2-C2	3.61	1.30	1.23
1	A	315	CFZ	O2-C2	3.61	1.30	1.23
1	B	15	CFZ	O2-C2	3.60	1.30	1.23
1	B	165	CFZ	O2-C2	3.60	1.30	1.23
1	B	354	CFZ	O2-C2	3.60	1.30	1.23
1	A	407	CFZ	O2-C2	3.60	1.30	1.23
1	B	474	CFZ	O2-C2	3.60	1.30	1.23
1	A	550	CFZ	O2-C2	3.60	1.30	1.23
1	A	664	CFZ	O2-C2	3.60	1.30	1.23
1	B	459	CFZ	O2-C2	3.60	1.30	1.23
1	B	517	CFZ	O2-C2	3.60	1.30	1.23
1	B	585	CFZ	O2-C2	3.60	1.30	1.23
1	B	610	CFZ	O2-C2	3.60	1.30	1.23
1	A	171	CFZ	O2-C2	3.60	1.30	1.23
1	B	655	CFZ	O2-C2	3.60	1.30	1.23
1	B	110	CFZ	O2-C2	3.60	1.30	1.23
1	B	96	CFZ	O2-C2	3.60	1.30	1.23
1	B	440	CFZ	O2-C2	3.60	1.30	1.23
1	B	399	CFZ	O2-C2	3.60	1.30	1.23
1	B	72	CFZ	O2-C2	3.60	1.30	1.23
1	A	316	CFZ	O2-C2	3.60	1.30	1.23
1	B	411	CFZ	O2-C2	3.60	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	498	CFZ	O2-C2	3.60	1.30	1.23
1	B	247	CFZ	O2-C2	3.60	1.30	1.23
1	A	473	CFZ	O2-C2	3.60	1.30	1.23
1	A	173	CFZ	O2-C2	3.60	1.30	1.23
1	B	551	CFZ	O2-C2	3.60	1.30	1.23
1	B	632	CFZ	O2-C2	3.60	1.30	1.23
1	A	298	CFZ	O2-C2	3.60	1.30	1.23
1	B	556	CFZ	O2-C2	3.60	1.30	1.23
1	A	647	CFZ	O2-C2	3.60	1.30	1.23
1	B	60	UFT	C2'-C3'	-3.60	1.47	1.52
1	A	114	CFZ	O2-C2	3.60	1.30	1.23
1	B	246	CFZ	O2-C2	3.60	1.30	1.23
1	A	399	CFZ	O2-C2	3.60	1.30	1.23
1	B	511	CFZ	O2-C2	3.60	1.30	1.23
1	B	439	CFZ	O2-C2	3.60	1.30	1.23
1	A	446	CFZ	O2-C2	3.60	1.30	1.23
1	B	583	CFZ	O2-C2	3.60	1.30	1.23
1	A	604	CFZ	O2-C2	3.60	1.30	1.23
1	A	140	CFZ	O2-C2	3.60	1.30	1.23
1	A	308	CFZ	O2-C2	3.60	1.30	1.23
1	A	144	CFZ	O2-C2	3.60	1.30	1.23
1	A	321	CFZ	O2-C2	3.60	1.30	1.23
1	A	444	CFZ	O2-C2	3.60	1.30	1.23
1	A	451	CFZ	O2-C2	3.60	1.30	1.23
1	A	657	CFZ	O2-C2	3.60	1.30	1.23
1	A	682	CFZ	O2-C2	3.60	1.30	1.23
1	B	26	CFZ	O2-C2	3.60	1.30	1.23
1	A	157	CFZ	O2-C2	3.60	1.30	1.23
1	A	73	CFZ	O2-C2	3.60	1.30	1.23
1	B	117	CFZ	O2-C2	3.60	1.30	1.23
1	B	637	CFZ	O2-C2	3.59	1.30	1.23
1	A	574	CFZ	O2-C2	3.59	1.30	1.23
1	B	592	CFZ	O2-C2	3.59	1.30	1.23
1	B	305	UFT	C2'-C3'	-3.59	1.47	1.52
1	A	165	CFZ	O2-C2	3.59	1.30	1.23
1	B	625	CFZ	O2-C2	3.59	1.30	1.23
1	A	643	CFZ	O2-C2	3.59	1.30	1.23
1	A	232	CFZ	O2-C2	3.59	1.30	1.23
1	A	234	CFZ	O2-C2	3.59	1.30	1.23
1	B	173	CFZ	O2-C2	3.59	1.30	1.23
1	A	372	CFZ	O2-C2	3.59	1.30	1.23
1	A	161	CFZ	O2-C2	3.59	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	587	CFZ	O2-C2	3.59	1.30	1.23
1	B	351	CFZ	O2-C2	3.59	1.30	1.23
1	B	639	CFZ	O2-C2	3.59	1.30	1.23
1	B	321	CFZ	O2-C2	3.59	1.30	1.23
1	A	543	CFZ	O2-C2	3.59	1.30	1.23
1	A	693	CFZ	O2-C2	3.59	1.30	1.23
1	A	458	CFZ	O2-C2	3.59	1.30	1.23
1	B	57	CFZ	O2-C2	3.59	1.30	1.23
1	A	469	CFZ	O2-C2	3.59	1.30	1.23
1	A	506	CFZ	O2-C2	3.59	1.30	1.23
1	A	164	CFZ	O2-C2	3.59	1.30	1.23
1	A	201	CFZ	O2-C2	3.59	1.30	1.23
1	A	417	CFZ	O2-C2	3.59	1.30	1.23
1	B	425	CFZ	O2-C2	3.59	1.30	1.23
1	B	576	CFZ	O2-C2	3.59	1.30	1.23
1	B	664	CFZ	O2-C2	3.59	1.30	1.23
1	A	268	CFZ	O2-C2	3.59	1.30	1.23
1	A	373	CFZ	O2-C2	3.59	1.30	1.23
1	B	249	CFZ	O2-C2	3.59	1.30	1.23
1	B	353	CFZ	O2-C2	3.59	1.30	1.23
1	B	518	CFZ	O2-C2	3.59	1.30	1.23
1	B	491	CFZ	O2-C2	3.59	1.30	1.23
1	B	564	CFZ	O2-C2	3.59	1.30	1.23
1	A	583	CFZ	O2-C2	3.59	1.30	1.23
1	B	647	CFZ	O2-C2	3.59	1.30	1.23
1	A	25	CFZ	O2-C2	3.59	1.30	1.23
1	A	404	CFZ	O2-C2	3.59	1.30	1.23
1	A	351	CFZ	O2-C2	3.58	1.30	1.23
1	B	373	CFZ	O2-C2	3.58	1.30	1.23
1	A	587	CFZ	O2-C2	3.58	1.30	1.23
1	B	328	CFZ	O2-C2	3.58	1.30	1.23
1	B	139	CFZ	O2-C2	3.58	1.30	1.23
1	B	282	CFZ	O2-C2	3.58	1.30	1.23
1	B	316	CFZ	O2-C2	3.58	1.30	1.23
1	A	614	CFZ	O2-C2	3.58	1.30	1.23
1	B	111	CFZ	O2-C2	3.58	1.30	1.23
1	B	206	CFZ	O2-C2	3.58	1.30	1.23
1	A	639	CFZ	O2-C2	3.58	1.30	1.23
1	A	218	CFZ	O2-C2	3.58	1.30	1.23
1	B	407	CFZ	O2-C2	3.58	1.30	1.23
1	B	631	CFZ	O2-C2	3.58	1.30	1.23
1	A	75	CFZ	O2-C2	3.58	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	CFZ	O2-C2	3.58	1.30	1.23
1	A	139	CFZ	O2-C2	3.58	1.30	1.23
1	B	469	CFZ	O2-C2	3.58	1.30	1.23
1	B	492	CFZ	O2-C2	3.58	1.30	1.23
1	A	72	CFZ	O2-C2	3.58	1.30	1.23
1	B	218	CFZ	O2-C2	3.58	1.30	1.23
1	A	209	CFZ	O2-C2	3.58	1.30	1.23
1	B	323	CFZ	O2-C2	3.58	1.30	1.23
1	B	372	CFZ	O2-C2	3.58	1.30	1.23
1	A	667	CFZ	O2-C2	3.58	1.30	1.23
1	A	679	CFZ	O2-C2	3.58	1.30	1.23
1	B	104	CFZ	O2-C2	3.58	1.30	1.23
1	B	25	CFZ	O2-C2	3.58	1.30	1.23
1	B	465	CFZ	O2-C2	3.58	1.30	1.23
1	A	15	CFZ	O2-C2	3.58	1.30	1.23
1	B	254	CFZ	O2-C2	3.57	1.30	1.23
1	A	486	CFZ	O2-C2	3.57	1.30	1.23
1	A	117	CFZ	O2-C2	3.57	1.30	1.23
1	B	219	CFZ	O2-C2	3.57	1.30	1.23
1	A	328	CFZ	O2-C2	3.57	1.30	1.23
1	A	576	CFZ	O2-C2	3.57	1.30	1.23
1	B	704	CFZ	O2-C2	3.57	1.30	1.23
1	B	63	CFZ	O2-C2	3.57	1.30	1.23
1	B	494	CFZ	O2-C2	3.57	1.30	1.23
1	A	637	CFZ	O2-C2	3.57	1.30	1.23
1	A	332	CFZ	O2-C2	3.57	1.30	1.23
1	A	363	CFZ	O2-C2	3.57	1.30	1.23
1	A	405	CFZ	O2-C2	3.57	1.30	1.23
1	A	438	CFZ	O2-C2	3.57	1.30	1.23
1	B	161	CFZ	O2-C2	3.57	1.30	1.23
1	A	426	CFZ	O2-C2	3.57	1.30	1.23
1	A	362	CFZ	O2-C2	3.57	1.30	1.23
1	B	544	UFT	C2'-C3'	-3.57	1.47	1.52
1	A	492	CFZ	O2-C2	3.57	1.30	1.23
1	B	473	CFZ	O2-C2	3.56	1.30	1.23
1	B	693	CFZ	O2-C2	3.56	1.30	1.23
1	A	512	CFZ	O2-C2	3.56	1.30	1.23
1	A	198	CFZ	O2-C2	3.56	1.30	1.23
1	B	201	CFZ	O2-C2	3.56	1.30	1.23
1	B	593	UFT	C2'-C3'	-3.56	1.47	1.52
1	A	536	CFZ	O2-C2	3.56	1.30	1.23
1	B	332	CFZ	O2-C2	3.56	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	CFZ	O2-C2	3.56	1.30	1.23
1	B	304	CFZ	O2-C2	3.56	1.30	1.23
1	B	171	CFZ	O2-C2	3.56	1.30	1.23
1	B	114	CFZ	O2-C2	3.56	1.30	1.23
1	A	57	CFZ	O2-C2	3.56	1.30	1.23
1	B	360	CFZ	O2-C2	3.56	1.30	1.23
1	B	446	CFZ	O2-C2	3.56	1.30	1.23
1	B	437	UFT	C2'-C3'	-3.56	1.47	1.52
1	A	111	CFZ	O2-C2	3.55	1.30	1.23
1	A	323	CFZ	O2-C2	3.55	1.30	1.23
1	A	378	CFZ	O2-C2	3.55	1.30	1.23
1	A	305	UFT	C2'-C3'	-3.55	1.47	1.52
1	B	383	CFZ	O2-C2	3.55	1.30	1.23
1	A	360	CFZ	O2-C2	3.55	1.30	1.23
1	A	632	CFZ	O2-C2	3.55	1.30	1.23
1	A	254	CFZ	O2-C2	3.55	1.30	1.23
1	B	124	CFZ	O2-C2	3.55	1.30	1.23
1	A	511	CFZ	O2-C2	3.55	1.30	1.23
1	A	60	UFT	C2'-C3'	-3.55	1.47	1.52
1	B	268	CFZ	O2-C2	3.55	1.30	1.23
1	A	124	CFZ	O2-C2	3.54	1.30	1.23
1	B	105	UFT	C2'-C3'	-3.54	1.47	1.52
1	A	76	CFZ	O2-C2	3.54	1.30	1.23
1	B	200	UFT	C2'-C3'	-3.54	1.47	1.52
1	B	657	CFZ	O2-C2	3.54	1.30	1.23
1	A	96	CFZ	O2-C2	3.53	1.30	1.23
1	A	657	CFZ	C2'-C3'	-3.52	1.47	1.52
1	A	13	UFT	C2'-C3'	-3.49	1.47	1.52
1	A	105	UFT	C2'-C3'	-3.49	1.47	1.52
1	B	606	UFT	C2'-C3'	-3.48	1.47	1.52
1	B	76	CFZ	O2-C2	3.48	1.30	1.23
1	A	437	UFT	C2'-C3'	-3.48	1.47	1.52
1	B	582	UFT	C2'-C3'	-3.48	1.47	1.52
1	A	606	UFT	C2'-C3'	-3.47	1.47	1.52
1	A	582	UFT	C2'-C3'	-3.43	1.47	1.52
1	B	657	CFZ	C2'-C3'	-3.38	1.48	1.52
1	B	494	CFZ	C2'-C1'	-3.37	1.48	1.53
1	B	491	CFZ	O4'-C1'	3.36	1.50	1.42
1	A	518	CFZ	C2'-C1'	-3.35	1.48	1.53
1	B	592	CFZ	O4'-C1'	3.32	1.49	1.42
1	A	200	UFT	C2'-C3'	-3.30	1.48	1.52
1	B	28	CFZ	O4'-C1'	3.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	CFZ	C2'-C1'	-3.27	1.48	1.53
1	A	355	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	39	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	354	CFZ	O4'-C1'	3.23	1.49	1.42
1	B	39	CFZ	O4'-C1'	3.23	1.49	1.42
1	B	492	CFZ	O4'-C1'	3.22	1.49	1.42
1	B	551	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	486	CFZ	O4'-C1'	3.21	1.49	1.42
1	B	25	CFZ	C2'-C1'	-3.21	1.48	1.53
1	B	316	CFZ	O4'-C1'	3.19	1.49	1.42
1	B	494	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	592	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	218	CFZ	O4'-C1'	3.19	1.49	1.42
1	B	247	CFZ	O4'-C1'	3.18	1.49	1.42
1	A	647	CFZ	O4'-C1'	3.18	1.49	1.42
1	A	551	CFZ	O4'-C1'	3.18	1.49	1.42
1	B	458	CFZ	C2'-C1'	-3.18	1.49	1.53
1	A	129	CFZ	O4'-C1'	3.18	1.49	1.42
1	A	455	CFZ	O4'-C1'	3.17	1.49	1.42
1	B	512	CFZ	O4'-C1'	3.17	1.49	1.42
1	B	682	CFZ	O4'-C1'	3.17	1.49	1.42
1	A	682	CFZ	O4'-C1'	3.17	1.49	1.42
1	B	49	CFZ	O4'-C1'	3.17	1.49	1.42
1	A	209	CFZ	O4'-C1'	3.17	1.49	1.42
1	B	362	CFZ	C2'-C1'	-3.17	1.49	1.53
1	B	129	CFZ	O4'-C1'	3.17	1.49	1.42
1	B	21	CFZ	O4'-C1'	3.17	1.49	1.42
1	A	156	CFZ	O4'-C1'	3.17	1.49	1.42
1	A	249	CFZ	O4'-C1'	3.17	1.49	1.42
1	A	279	CFZ	O4'-C1'	3.17	1.49	1.42
1	B	698	CFZ	O4'-C1'	3.17	1.49	1.42
1	A	568	CFZ	O4'-C1'	3.16	1.49	1.42
1	B	550	CFZ	O4'-C1'	3.16	1.49	1.42
1	A	130	CFZ	O4'-C1'	3.16	1.49	1.42
1	B	565	CFZ	C2'-C1'	-3.16	1.49	1.53
1	B	120	CFZ	O4'-C1'	3.16	1.49	1.42
1	B	568	CFZ	O4'-C1'	3.16	1.49	1.42
1	B	246	CFZ	O4'-C1'	3.16	1.49	1.42
1	A	46	CFZ	O4'-C1'	3.16	1.49	1.42
1	A	165	CFZ	O4'-C1'	3.16	1.49	1.42
1	A	446	CFZ	C2'-C1'	-3.16	1.49	1.53
1	A	512	CFZ	O4'-C1'	3.15	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	315	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	587	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	441	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	574	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	46	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	316	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	647	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	219	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	285	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	362	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	363	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	600	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	188	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	383	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	446	CFZ	C2'-C1'	-3.15	1.49	1.53
1	A	28	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	209	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	304	CFZ	O4'-C1'	3.15	1.49	1.42
1	B	165	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	498	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	600	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	587	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	631	CFZ	C2'-C1'	-3.14	1.49	1.53
1	A	184	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	494	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	614	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	406	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	219	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	315	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	604	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	285	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	387	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	679	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	120	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	72	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	184	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	282	CFZ	C2'-C1'	-3.14	1.49	1.53
1	B	130	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	424	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	465	CFZ	O4'-C1'	3.14	1.49	1.42
1	B	370	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	528	CFZ	O4'-C1'	3.14	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	459	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	34	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	149	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	652	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	49	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	139	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	218	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	550	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	540	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	372	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	157	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	425	CFZ	C2'-C1'	-3.13	1.49	1.53
1	A	698	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	21	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	458	CFZ	C2'-C1'	-3.13	1.49	1.53
1	A	157	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	298	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	528	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	424	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	298	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	279	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	72	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	425	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	355	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	436	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	67	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	304	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	156	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	131	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	104	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	441	CFZ	O4'-C1'	3.13	1.49	1.42
1	B	323	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	565	CFZ	C2'-C1'	-3.13	1.49	1.53
1	B	131	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	369	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	614	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	124	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	693	CFZ	O4'-C1'	3.12	1.49	1.42
1	B	576	CFZ	C2'-C1'	-3.12	1.49	1.53
1	B	446	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	474	CFZ	O4'-C1'	3.12	1.49	1.42
1	B	574	CFZ	O4'-C1'	3.12	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	576	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	462	CFZ	O4'-C1'	3.12	1.49	1.42
1	B	511	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	378	CFZ	O4'-C1'	3.12	1.49	1.42
1	B	693	CFZ	O4'-C1'	3.12	1.49	1.42
1	B	188	CFZ	O4'-C1'	3.12	1.49	1.42
1	B	406	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	246	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	632	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	652	CFZ	O4'-C1'	3.12	1.49	1.42
1	B	111	CFZ	C2'-C1'	-3.12	1.49	1.53
1	B	249	CFZ	O4'-C1'	3.12	1.49	1.42
1	B	643	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	425	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	10	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	96	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	387	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	458	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	325	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	407	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	540	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	232	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	242	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	173	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	111	CFZ	C2'-C1'	-3.11	1.49	1.53
1	A	411	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	198	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	458	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	370	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	498	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	151	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	247	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	579	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	363	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	446	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	459	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	679	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	360	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	657	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	383	CFZ	C2'-C1'	-3.11	1.49	1.53
1	A	57	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	149	CFZ	O4'-C1'	3.11	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	604	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	104	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	632	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	73	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	700	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	206	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	405	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	411	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	351	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	418	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	465	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	418	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	473	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	477	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	404	CFZ	O4'-C1'	3.11	1.49	1.42
1	B	548	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	565	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	451	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	491	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	603	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	603	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	173	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	399	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	558	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	704	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	161	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	383	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	651	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	34	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	44	UFT	O4-C4	-3.10	1.18	1.24
1	B	372	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	325	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	373	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	523	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	57	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	349	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	381	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	511	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	548	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	378	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	151	CFZ	O4'-C1'	3.10	1.49	1.42
1	B	139	CFZ	O4'-C1'	3.10	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	700	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	576	CFZ	C2'-C1'	-3.10	1.49	1.53
1	B	426	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	323	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	362	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	124	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	517	CFZ	C2'-C1'	-3.09	1.49	1.53
1	A	579	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	282	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	517	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	647	CFZ	C2'-C1'	-3.09	1.49	1.53
1	B	79	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	407	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	381	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	506	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	335	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	201	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	73	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	576	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	242	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	426	CFZ	O4'-C1'	3.09	1.49	1.42
1	A	425	CFZ	C2'-C1'	-3.09	1.49	1.53
1	B	201	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	206	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	76	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	103	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	631	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	161	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	585	CFZ	O4'-C1'	3.09	1.49	1.42
1	B	506	CFZ	O4'-C1'	3.08	1.49	1.42
1	B	164	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	254	CFZ	O4'-C1'	3.08	1.49	1.42
1	B	474	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	631	CFZ	C2'-C1'	-3.08	1.49	1.53
1	B	198	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	643	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	405	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	164	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	335	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	404	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	565	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	631	CFZ	O4'-C1'	3.08	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	704	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	79	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	76	CFZ	O4'-C1'	3.08	1.49	1.42
1	B	486	CFZ	O4'-C1'	3.08	1.49	1.42
1	B	657	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	492	CFZ	O4'-C1'	3.08	1.49	1.42
1	B	492	CFZ	C2'-C1'	-3.08	1.49	1.53
1	A	691	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	536	CFZ	O4'-C1'	3.08	1.49	1.42
1	B	332	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	140	CFZ	O4'-C1'	3.07	1.49	1.42
1	B	417	CFZ	O4'-C1'	3.07	1.49	1.42
1	B	111	CFZ	O4'-C1'	3.07	1.49	1.42
1	B	373	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	620	CFZ	O4'-C1'	3.07	1.49	1.42
1	B	369	CFZ	O4'-C1'	3.07	1.49	1.42
1	B	564	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	439	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	625	CFZ	O4'-C1'	3.07	1.49	1.42
1	B	140	CFZ	O4'-C1'	3.07	1.49	1.42
1	B	440	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	518	CFZ	O4'-C1'	3.07	1.49	1.42
1	B	625	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	426	CFZ	C2'-C1'	-3.07	1.49	1.53
1	B	110	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	111	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	384	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	338	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	268	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	399	CFZ	O4'-C1'	3.07	1.49	1.42
1	B	254	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	477	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	651	CFZ	O4'-C1'	3.07	1.49	1.42
1	A	417	CFZ	O4'-C1'	3.06	1.49	1.42
1	B	439	CFZ	O4'-C1'	3.06	1.49	1.42
1	B	551	CFZ	C2'-C1'	-3.06	1.49	1.53
1	B	212	CFZ	O4'-C1'	3.06	1.49	1.42
1	A	282	CFZ	O4'-C1'	3.06	1.49	1.42
1	A	282	CFZ	C2'-C1'	-3.06	1.49	1.53
1	A	363	CFZ	C2'-C1'	-3.06	1.49	1.53
1	B	354	CFZ	O4'-C1'	3.06	1.49	1.42
1	B	655	CFZ	O4'-C1'	3.06	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	543	CFZ	O4'-C1'	3.06	1.49	1.42
1	A	321	CFZ	O4'-C1'	3.06	1.49	1.42
1	A	440	CFZ	O4'-C1'	3.06	1.49	1.42
1	B	268	CFZ	O4'-C1'	3.06	1.49	1.42
1	B	639	CFZ	O4'-C1'	3.06	1.49	1.42
1	B	247	CFZ	C2'-C1'	-3.06	1.49	1.53
1	A	26	CFZ	O4'-C1'	3.06	1.49	1.42
1	A	351	CFZ	O4'-C1'	3.06	1.49	1.42
1	A	469	CFZ	O4'-C1'	3.06	1.49	1.42
1	B	610	CFZ	O4'-C1'	3.06	1.49	1.42
1	B	620	CFZ	O4'-C1'	3.06	1.49	1.42
1	A	110	CFZ	O4'-C1'	3.05	1.49	1.42
1	A	585	CFZ	O4'-C1'	3.05	1.49	1.42
1	B	338	CFZ	O4'-C1'	3.05	1.49	1.42
1	B	473	CFZ	O4'-C1'	3.05	1.49	1.42
1	A	302	UFT	O4-C4	-3.05	1.18	1.24
1	B	438	CFZ	O4'-C1'	3.05	1.49	1.42
1	A	103	CFZ	O4'-C1'	3.05	1.49	1.42
1	B	518	CFZ	O4'-C1'	3.05	1.49	1.42
1	B	353	CFZ	O4'-C1'	3.05	1.49	1.42
1	B	477	CFZ	C2'-C1'	-3.05	1.49	1.53
1	B	558	CFZ	O4'-C1'	3.05	1.49	1.42
1	A	477	CFZ	C2'-C1'	-3.05	1.49	1.53
1	B	691	CFZ	O4'-C1'	3.05	1.49	1.42
1	A	564	CFZ	O4'-C1'	3.05	1.49	1.42
1	B	302	UFT	O4-C4	-3.05	1.18	1.24
1	A	610	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	639	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	444	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	517	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	436	CFZ	C2'-C1'	-3.04	1.49	1.53
1	B	241	CFZ	O4'-C1'	3.04	1.49	1.42
1	B	75	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	332	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	543	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	362	CFZ	C2'-C1'	-3.03	1.49	1.53
1	B	469	CFZ	O4'-C1'	3.03	1.49	1.42
1	A	667	CFZ	O4'-C1'	3.03	1.49	1.42
1	B	667	CFZ	O4'-C1'	3.03	1.49	1.42
1	B	363	CFZ	C2'-C1'	-3.03	1.49	1.53
1	A	655	CFZ	O4'-C1'	3.03	1.49	1.42
1	B	232	CFZ	O4'-C1'	3.03	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	CFZ	O4'-C1'	3.03	1.49	1.42
1	A	25	CFZ	O4'-C1'	3.03	1.49	1.42
1	B	523	CFZ	O4'-C1'	3.03	1.49	1.42
1	B	96	CFZ	O4'-C1'	3.03	1.49	1.42
1	B	25	CFZ	O4'-C1'	3.03	1.49	1.42
1	B	655	CFZ	C2'-C1'	-3.02	1.49	1.53
1	B	63	CFZ	O4'-C1'	3.02	1.49	1.42
1	A	315	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	556	CFZ	O4'-C1'	3.02	1.49	1.42
1	B	637	CFZ	O4'-C1'	3.02	1.49	1.42
1	B	511	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	308	CFZ	O4'-C1'	3.02	1.49	1.42
1	A	210	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	637	CFZ	O4'-C1'	3.02	1.49	1.42
1	B	26	CFZ	O4'-C1'	3.02	1.49	1.42
1	B	210	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	511	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	209	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	492	CFZ	C2'-C1'	-3.02	1.49	1.53
1	B	171	CFZ	O4'-C1'	3.02	1.49	1.42
1	A	57	CFZ	C2'-C1'	-3.02	1.49	1.53
1	B	361	UFT	O4-C4	-3.02	1.18	1.24
1	A	212	CFZ	O4'-C1'	3.02	1.49	1.42
1	A	114	CFZ	O4'-C1'	3.02	1.49	1.42
1	B	372	CFZ	C2'-C1'	-3.02	1.49	1.53
1	B	308	CFZ	O4'-C1'	3.02	1.49	1.42
1	A	328	CFZ	O4'-C1'	3.02	1.49	1.42
1	B	234	CFZ	O4'-C1'	3.02	1.49	1.42
1	A	438	CFZ	O4'-C1'	3.02	1.49	1.42
1	B	67	CFZ	O4'-C1'	3.01	1.49	1.42
1	B	536	CFZ	O4'-C1'	3.01	1.49	1.42
1	A	63	CFZ	O4'-C1'	3.01	1.49	1.42
1	B	556	CFZ	O4'-C1'	3.01	1.49	1.42
1	A	104	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	124	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	171	CFZ	O4'-C1'	3.01	1.49	1.42
1	B	315	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	556	CFZ	C2'-C1'	-3.01	1.49	1.53
1	B	647	CFZ	C2'-C1'	-3.01	1.49	1.53
1	B	104	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	75	CFZ	O4'-C1'	3.01	1.49	1.42
1	B	321	CFZ	O4'-C1'	3.01	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	CFZ	O4'-C1'	3.01	1.49	1.42
1	A	372	CFZ	C2'-C1'	-3.00	1.49	1.53
1	B	76	CFZ	C2'-C1'	-3.00	1.49	1.53
1	B	10	CFZ	C2'-C1'	-3.00	1.49	1.53
1	B	114	CFZ	O4'-C1'	3.00	1.49	1.42
1	B	426	CFZ	C2'-C1'	-3.00	1.49	1.53
1	B	164	CFZ	C2'-C1'	-3.00	1.49	1.53
1	A	234	CFZ	C2'-C1'	-3.00	1.49	1.53
1	A	417	CFZ	C2'-C1'	-3.00	1.49	1.53
1	B	144	CFZ	O4'-C1'	3.00	1.49	1.42
1	B	664	CFZ	O4'-C1'	3.00	1.49	1.42
1	B	583	CFZ	O4'-C1'	2.99	1.49	1.42
1	B	361	UFT	C2'-C1'	-2.99	1.49	1.53
1	B	117	CFZ	O4'-C1'	2.99	1.49	1.42
1	A	234	CFZ	O4'-C1'	2.99	1.49	1.42
1	A	241	CFZ	O4'-C1'	2.99	1.49	1.42
1	B	518	CFZ	C2'-C1'	-2.99	1.49	1.53
1	B	643	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	164	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	144	CFZ	O4'-C1'	2.99	1.49	1.42
1	A	664	CFZ	O4'-C1'	2.99	1.49	1.42
1	B	218	CFZ	C2'-C1'	-2.99	1.49	1.53
1	B	234	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	583	CFZ	O4'-C1'	2.99	1.49	1.42
1	A	98	UFT	O4-C4	-2.99	1.18	1.24
1	B	417	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	378	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	44	UFT	O4-C4	-2.99	1.18	1.24
1	B	165	CFZ	C2'-C1'	-2.98	1.49	1.53
1	B	459	CFZ	C2'-C1'	-2.98	1.49	1.53
1	A	249	CFZ	C2'-C1'	-2.98	1.49	1.53
1	A	432	UFT	O4-C4	-2.98	1.18	1.24
1	A	39	CFZ	C2'-C1'	-2.98	1.49	1.53
1	A	558	CFZ	C2'-C1'	-2.98	1.49	1.53
1	A	568	CFZ	C2'-C1'	-2.98	1.49	1.53
1	B	384	CFZ	O4'-C1'	2.98	1.49	1.42
1	B	21	CFZ	C2'-C1'	-2.98	1.49	1.53
1	B	512	CFZ	C2'-C1'	-2.98	1.49	1.53
1	A	550	CFZ	C2'-C1'	-2.98	1.49	1.53
1	B	360	CFZ	O4'-C1'	2.97	1.49	1.42
1	A	173	CFZ	C2'-C1'	-2.97	1.49	1.53
1	B	352	UFT	O4-C4	-2.97	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	632	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	459	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	353	CFZ	O4'-C1'	2.97	1.49	1.42
1	B	46	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	321	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	210	CFZ	O4'-C1'	2.97	1.49	1.42
1	B	206	CFZ	C2'-C1'	-2.97	1.49	1.53
1	B	90	CFZ	O4'-C1'	2.97	1.49	1.42
1	B	124	CFZ	C2'-C1'	-2.97	1.49	1.53
1	B	209	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	523	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	350	UFT	O4-C4	-2.97	1.18	1.24
1	B	173	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	387	CFZ	C2'-C1'	-2.96	1.49	1.53
1	A	15	CFZ	O4'-C1'	2.96	1.49	1.42
1	B	210	CFZ	O4'-C1'	2.96	1.49	1.42
1	A	21	CFZ	C2'-C1'	-2.96	1.49	1.53
1	B	184	CFZ	C2'-C1'	-2.96	1.49	1.53
1	B	328	CFZ	O4'-C1'	2.96	1.49	1.42
1	B	556	CFZ	C2'-C1'	-2.96	1.49	1.53
1	A	165	CFZ	C2'-C1'	-2.96	1.49	1.53
1	A	655	CFZ	C2'-C1'	-2.96	1.49	1.53
1	B	129	CFZ	C2'-C1'	-2.96	1.49	1.53
1	B	387	CFZ	C2'-C1'	-2.96	1.49	1.53
1	B	698	CFZ	C2'-C1'	-2.96	1.49	1.53
1	A	218	CFZ	C2'-C1'	-2.95	1.49	1.53
1	B	49	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	206	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	46	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	229	UFT	O4-C4	-2.95	1.18	1.24
1	A	270	UFT	O4-C4	-2.95	1.18	1.24
1	A	90	CFZ	O4'-C1'	2.95	1.49	1.42
1	A	149	CFZ	C2'-C1'	-2.95	1.49	1.53
1	B	689	UFT	O4-C4	-2.95	1.18	1.24
1	A	413	UFT	O4-C4	-2.95	1.18	1.24
1	A	76	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	370	CFZ	C2'-C1'	-2.95	1.49	1.53
1	B	246	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	551	CFZ	C2'-C1'	-2.95	1.49	1.53
1	B	636	UFT	O4-C4	-2.95	1.18	1.24
1	A	489	UFT	O4-C4	-2.95	1.18	1.24
1	A	662	UFT	O4-C4	-2.94	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	456	UFT	O4-C4	-2.94	1.18	1.24
1	A	84	UFT	O4-C4	-2.94	1.18	1.24
1	B	535	UFT	O4-C4	-2.94	1.18	1.24
1	B	39	CFZ	C2'-C1'	-2.94	1.49	1.53
1	B	142	UFT	O4-C4	-2.94	1.18	1.24
1	B	175	UFT	O4-C4	-2.94	1.18	1.24
1	B	432	UFT	O4-C4	-2.94	1.18	1.24
1	B	75	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	304	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	643	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	72	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	88	UFT	O4-C4	-2.94	1.18	1.24
1	A	116	UFT	O4-C4	-2.94	1.18	1.24
1	A	265	UFT	O4-C4	-2.94	1.18	1.24
1	A	659	UFT	O4-C4	-2.94	1.18	1.24
1	B	15	CFZ	O4'-C1'	2.94	1.49	1.42
1	A	693	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	59	UFT	O4-C4	-2.94	1.18	1.24
1	B	98	UFT	O4-C4	-2.94	1.18	1.24
1	B	304	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	48	UFT	O4-C4	-2.94	1.18	1.24
1	A	112	UFT	O4-C4	-2.94	1.18	1.24
1	B	283	UFT	O4-C4	-2.94	1.18	1.24
1	B	103	CFZ	C2'-C1'	-2.94	1.49	1.53
1	B	389	UFT	O4-C4	-2.94	1.18	1.24
1	B	249	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	571	UFT	O4-C4	-2.94	1.18	1.24
1	A	460	UFT	O4-C4	-2.94	1.18	1.24
1	B	524	UFT	O4-C4	-2.94	1.18	1.24
1	B	154	UFT	O4-C4	-2.93	1.18	1.24
1	B	321	CFZ	C2'-C1'	-2.93	1.49	1.53
1	B	42	UFT	O4-C4	-2.93	1.18	1.24
1	B	192	UFT	O4-C4	-2.93	1.18	1.24
1	A	192	UFT	O4-C4	-2.93	1.18	1.24
1	B	270	UFT	O4-C4	-2.93	1.18	1.24
1	A	554	UFT	O4-C4	-2.93	1.18	1.24
1	A	581	UFT	O4-C4	-2.93	1.18	1.24
1	A	534	UFT	O4-C4	-2.93	1.18	1.24
1	B	581	UFT	O4-C4	-2.93	1.18	1.24
1	B	96	CFZ	C2'-C1'	-2.93	1.49	1.53
1	B	336	UFT	O4-C4	-2.93	1.18	1.24
1	A	367	UFT	O4-C4	-2.93	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	367	UFT	O4-C4	-2.93	1.18	1.24
1	B	720	UFT	O4-C4	-2.93	1.18	1.24
1	A	673	UFT	O4-C4	-2.93	1.18	1.24
1	A	157	CFZ	C2'-C1'	-2.93	1.49	1.53
1	A	32	UFT	O4-C4	-2.93	1.18	1.24
1	B	447	UFT	O4-C4	-2.93	1.18	1.24
1	A	549	UFT	O4-C4	-2.93	1.18	1.24
1	B	568	CFZ	C2'-C1'	-2.93	1.49	1.53
1	B	309	UFT	O4-C4	-2.93	1.18	1.24
1	A	251	UFT	O4-C4	-2.93	1.18	1.24
1	B	402	UFT	O4-C4	-2.93	1.18	1.24
1	B	695	UFT	O4-C4	-2.93	1.18	1.24
1	A	215	UFT	O4-C4	-2.93	1.18	1.24
1	A	344	UFT	O4-C4	-2.93	1.18	1.24
1	B	460	UFT	O4-C4	-2.93	1.18	1.24
1	B	549	UFT	O4-C4	-2.93	1.18	1.24
1	A	577	UFT	O4-C4	-2.93	1.18	1.24
1	B	690	UFT	O4-C4	-2.93	1.18	1.24
1	A	69	UFT	O4-C4	-2.93	1.18	1.24
1	A	154	UFT	O4-C4	-2.93	1.18	1.24
1	A	676	UFT	O4-C4	-2.93	1.18	1.24
1	B	112	UFT	O4-C4	-2.93	1.18	1.24
1	B	712	UFT	O4-C4	-2.93	1.18	1.24
1	B	215	UFT	O4-C4	-2.93	1.18	1.24
1	B	464	UFT	O4-C4	-2.93	1.18	1.24
1	A	602	UFT	O4-C4	-2.93	1.18	1.24
1	A	67	CFZ	C2'-C1'	-2.93	1.49	1.53
1	A	188	CFZ	C2'-C1'	-2.93	1.49	1.53
1	B	10	CFZ	O4'-C1'	2.93	1.48	1.42
1	A	309	UFT	O4-C4	-2.93	1.18	1.24
1	B	593	UFT	O4-C4	-2.93	1.18	1.24
1	B	602	UFT	O4-C4	-2.93	1.18	1.24
1	A	352	UFT	O4-C4	-2.93	1.18	1.24
1	B	421	UFT	O4-C4	-2.93	1.18	1.24
1	A	590	UFT	O4-C4	-2.93	1.18	1.24
1	A	49	CFZ	C2'-C1'	-2.93	1.49	1.53
1	B	405	CFZ	C2'-C1'	-2.93	1.49	1.53
1	A	451	CFZ	C2'-C1'	-2.93	1.49	1.53
1	B	200	UFT	O4-C4	-2.93	1.18	1.24
1	B	656	UFT	O4-C4	-2.93	1.18	1.24
1	B	110	CFZ	C2'-C1'	-2.93	1.49	1.53
1	A	512	CFZ	C2'-C1'	-2.93	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	682	CFZ	C2'-C1'	-2.93	1.49	1.53
1	B	170	UFT	O4-C4	-2.93	1.18	1.24
1	B	365	UFT	O4-C4	-2.93	1.18	1.24
1	A	71	UFT	O4-C4	-2.92	1.18	1.24
1	B	84	UFT	O4-C4	-2.92	1.18	1.24
1	B	489	UFT	O4-C4	-2.92	1.18	1.24
1	A	329	UFT	O4-C4	-2.92	1.18	1.24
1	A	431	UFT	O4-C4	-2.92	1.18	1.24
1	A	712	UFT	O4-C4	-2.92	1.18	1.24
1	A	74	UFT	O4-C4	-2.92	1.18	1.24
1	B	296	UFT	O4-C4	-2.92	1.18	1.24
1	B	603	CFZ	C2'-C1'	-2.92	1.49	1.53
1	B	265	UFT	O4-C4	-2.92	1.18	1.24
1	A	481	UFT	O4-C4	-2.92	1.18	1.24
1	B	499	UFT	O4-C4	-2.92	1.18	1.24
1	A	336	UFT	O4-C4	-2.92	1.18	1.24
1	A	73	CFZ	C2'-C1'	-2.92	1.49	1.53
1	A	298	CFZ	C2'-C1'	-2.92	1.49	1.53
1	B	632	CFZ	C2'-C1'	-2.92	1.49	1.53
1	A	403	UFT	O4-C4	-2.92	1.18	1.24
1	A	696	UFT	O4-C4	-2.92	1.18	1.24
1	B	242	CFZ	C2'-C1'	-2.92	1.49	1.53
1	A	698	CFZ	C2'-C1'	-2.92	1.49	1.53
1	B	571	UFT	O4-C4	-2.92	1.18	1.24
1	A	719	UFT	O4-C4	-2.92	1.18	1.24
1	B	115	UFT	O4-C4	-2.92	1.18	1.24
1	A	509	UFT	O4-C4	-2.92	1.18	1.24
1	B	32	UFT	O4-C4	-2.92	1.18	1.24
1	A	266	UFT	O4-C4	-2.92	1.18	1.24
1	B	513	UFT	O4-C4	-2.92	1.18	1.24
1	B	534	UFT	O4-C4	-2.92	1.18	1.24
1	A	653	UFT	O4-C4	-2.92	1.18	1.24
1	A	105	UFT	O4-C4	-2.92	1.18	1.24
1	B	202	UFT	O4-C4	-2.92	1.18	1.24
1	A	635	UFT	O4-C4	-2.92	1.18	1.24
1	A	669	UFT	O4-C4	-2.92	1.18	1.24
1	A	8	UFT	O4-C4	-2.92	1.18	1.24
1	B	101	UFT	O4-C4	-2.92	1.18	1.24
1	B	398	UFT	O4-C4	-2.92	1.18	1.24
1	A	430	UFT	O4-C4	-2.92	1.18	1.24
1	A	608	UFT	O4-C4	-2.92	1.18	1.24
1	B	646	UFT	O4-C4	-2.92	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	700	CFZ	C2'-C1'	-2.92	1.49	1.53
1	A	115	UFT	O4-C4	-2.92	1.18	1.24
1	B	163	UFT	O4-C4	-2.92	1.18	1.24
1	B	214	UFT	O4-C4	-2.92	1.18	1.24
1	B	403	UFT	O4-C4	-2.92	1.18	1.24
1	B	431	UFT	O4-C4	-2.92	1.18	1.24
1	B	693	CFZ	C2'-C1'	-2.92	1.49	1.53
1	A	684	UFT	O4-C4	-2.92	1.18	1.24
1	B	62	UFT	O4-C4	-2.92	1.18	1.24
1	A	89	UFT	O4-C4	-2.92	1.18	1.24
1	B	359	UFT	O4-C4	-2.92	1.18	1.24
1	B	285	CFZ	C2'-C1'	-2.92	1.49	1.53
1	B	378	CFZ	C2'-C1'	-2.92	1.49	1.53
1	B	550	CFZ	C2'-C1'	-2.92	1.49	1.53
1	A	499	UFT	O4-C4	-2.92	1.18	1.24
1	A	559	UFT	O4-C4	-2.92	1.18	1.24
1	B	606	UFT	O4-C4	-2.92	1.18	1.24
1	B	621	UFT	O4-C4	-2.92	1.18	1.24
1	A	377	UFT	O4-C4	-2.92	1.18	1.24
1	A	389	UFT	O4-C4	-2.92	1.18	1.24
1	A	423	UFT	O4-C4	-2.92	1.18	1.24
1	A	142	UFT	O4-C4	-2.92	1.18	1.24
1	A	245	UFT	O4-C4	-2.92	1.18	1.24
1	B	628	UFT	O4-C4	-2.92	1.18	1.24
1	B	97	UFT	O4-C4	-2.92	1.18	1.24
1	B	153	UFT	O4-C4	-2.92	1.18	1.24
1	B	687	UFT	O4-C4	-2.92	1.18	1.24
1	A	689	UFT	O4-C4	-2.92	1.18	1.24
1	B	301	UFT	O4-C4	-2.91	1.18	1.24
1	A	471	UFT	O4-C4	-2.91	1.18	1.24
1	A	618	UFT	O4-C4	-2.91	1.18	1.24
1	A	14	UFT	O4-C4	-2.91	1.18	1.24
1	B	347	UFT	O4-C4	-2.91	1.18	1.24
1	A	472	UFT	O4-C4	-2.91	1.18	1.24
1	A	535	UFT	O4-C4	-2.91	1.18	1.24
1	B	629	UFT	O4-C4	-2.91	1.18	1.24
1	B	8	UFT	O4-C4	-2.91	1.18	1.24
1	B	33	UFT	O4-C4	-2.91	1.18	1.24
1	B	126	UFT	O4-C4	-2.91	1.18	1.24
1	A	296	UFT	O4-C4	-2.91	1.18	1.24
1	B	334	UFT	O4-C4	-2.91	1.18	1.24
1	B	607	UFT	O4-C4	-2.91	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	472	UFT	O4-C4	-2.91	1.18	1.24
1	A	524	UFT	O4-C4	-2.91	1.18	1.24
1	A	701	UFT	O4-C4	-2.91	1.18	1.24
1	B	14	UFT	O4-C4	-2.91	1.18	1.24
1	B	519	UFT	O4-C4	-2.91	1.18	1.24
1	A	609	UFT	O4-C4	-2.91	1.18	1.24
1	A	663	UFT	O4-C4	-2.91	1.18	1.24
1	A	33	UFT	O4-C4	-2.91	1.18	1.24
1	B	135	UFT	O4-C4	-2.91	1.18	1.24
1	B	179	UFT	O4-C4	-2.91	1.18	1.24
1	A	233	UFT	O4-C4	-2.91	1.18	1.24
1	B	437	UFT	O4-C4	-2.91	1.18	1.24
1	B	509	UFT	O4-C4	-2.91	1.18	1.24
1	A	582	UFT	O4-C4	-2.91	1.18	1.24
1	B	676	UFT	O4-C4	-2.91	1.18	1.24
1	B	80	UFT	O4-C4	-2.91	1.18	1.24
1	B	504	UFT	O4-C4	-2.91	1.18	1.24
1	A	607	UFT	O4-C4	-2.91	1.18	1.24
1	B	188	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	328	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	587	CFZ	C2'-C1'	-2.91	1.49	1.53
1	B	11	UFT	O4-C4	-2.91	1.18	1.24
1	A	169	UFT	O4-C4	-2.91	1.18	1.24
1	A	214	UFT	O4-C4	-2.91	1.18	1.24
1	B	229	UFT	O4-C4	-2.91	1.18	1.24
1	B	500	UFT	O4-C4	-2.91	1.18	1.24
1	B	530	UFT	O4-C4	-2.91	1.18	1.24
1	A	687	UFT	O4-C4	-2.91	1.18	1.24
1	B	399	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	528	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	50	UFT	O4-C4	-2.91	1.18	1.24
1	B	137	UFT	O4-C4	-2.91	1.18	1.24
1	B	430	UFT	O4-C4	-2.91	1.18	1.24
1	A	500	UFT	O4-C4	-2.91	1.18	1.24
1	A	293	UFT	O4-C4	-2.91	1.18	1.24
1	A	143	UFT	O4-C4	-2.91	1.18	1.24
1	A	555	UFT	O4-C4	-2.91	1.18	1.24
1	B	55	UFT	O4-C4	-2.91	1.18	1.24
1	A	202	UFT	O4-C4	-2.91	1.18	1.24
1	A	358	UFT	O4-C4	-2.91	1.18	1.24
1	B	542	UFT	O4-C4	-2.91	1.18	1.24
1	A	629	UFT	O4-C4	-2.91	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	633	UFT	O4-C4	-2.91	1.18	1.24
1	A	129	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	381	CFZ	C2'-C1'	-2.91	1.49	1.53
1	B	157	CFZ	C2'-C1'	-2.91	1.49	1.53
1	B	74	UFT	O4-C4	-2.91	1.18	1.24
1	B	106	UFT	O4-C4	-2.91	1.18	1.24
1	A	703	UFT	O4-C4	-2.91	1.18	1.24
1	A	153	UFT	O4-C4	-2.91	1.18	1.24
1	B	197	UFT	O4-C4	-2.91	1.18	1.24
1	A	593	UFT	O4-C4	-2.91	1.18	1.24
1	A	316	CFZ	C2'-C1'	-2.91	1.49	1.53
1	B	434	UFT	O4-C4	-2.91	1.18	1.24
1	B	666	UFT	O4-C4	-2.91	1.18	1.24
1	A	247	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	455	CFZ	C2'-C1'	-2.91	1.49	1.53
1	B	86	UFT	O4-C4	-2.91	1.18	1.24
1	A	106	UFT	O4-C4	-2.91	1.18	1.24
1	B	116	UFT	O4-C4	-2.91	1.18	1.24
1	A	184	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	285	CFZ	C2'-C1'	-2.91	1.49	1.53
1	B	673	UFT	O4-C4	-2.91	1.18	1.24
1	B	43	UFT	O4-C4	-2.90	1.18	1.24
1	A	519	UFT	O4-C4	-2.90	1.18	1.24
1	B	50	UFT	O4-C4	-2.90	1.18	1.24
1	A	545	UFT	O4-C4	-2.90	1.18	1.24
1	A	11	UFT	O4-C4	-2.90	1.18	1.24
1	B	108	UFT	O4-C4	-2.90	1.18	1.24
1	A	141	UFT	O4-C4	-2.90	1.18	1.24
1	A	365	UFT	O4-C4	-2.90	1.18	1.24
1	B	590	UFT	O4-C4	-2.90	1.18	1.24
1	A	323	CFZ	C2'-C1'	-2.90	1.49	1.53
1	B	48	UFT	O4-C4	-2.90	1.18	1.24
1	A	108	UFT	O4-C4	-2.90	1.18	1.24
1	A	464	UFT	O4-C4	-2.90	1.18	1.24
1	A	466	UFT	O4-C4	-2.90	1.18	1.24
1	B	684	UFT	O4-C4	-2.90	1.18	1.24
1	B	216	UFT	O4-C4	-2.90	1.18	1.24
1	B	423	UFT	O4-C4	-2.90	1.18	1.24
1	B	471	UFT	O4-C4	-2.90	1.18	1.24
1	A	513	UFT	O4-C4	-2.90	1.18	1.24
1	A	43	UFT	O4-C4	-2.90	1.18	1.24
1	A	61	UFT	O4-C4	-2.90	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	UFT	O4-C4	-2.90	1.18	1.24
1	A	200	UFT	O4-C4	-2.90	1.18	1.24
1	A	434	UFT	O4-C4	-2.90	1.18	1.24
1	A	666	UFT	O4-C4	-2.90	1.18	1.24
1	A	190	UFT	O4-C4	-2.90	1.18	1.24
1	A	216	UFT	O4-C4	-2.90	1.18	1.24
1	A	197	UFT	O4-C4	-2.90	1.18	1.24
1	A	398	UFT	O4-C4	-2.90	1.18	1.24
1	A	406	CFZ	C2'-C1'	-2.90	1.49	1.53
1	A	160	UFT	O4-C4	-2.90	1.18	1.24
1	B	251	UFT	O4-C4	-2.90	1.18	1.24
1	A	485	UFT	O4-C4	-2.90	1.18	1.24
1	B	174	UFT	O4-C4	-2.90	1.18	1.24
1	A	383	CFZ	C2'-C1'	-2.90	1.49	1.53
1	B	60	UFT	O4-C4	-2.90	1.18	1.24
1	B	544	UFT	O4-C4	-2.90	1.18	1.24
1	A	42	UFT	O4-C4	-2.90	1.18	1.24
1	B	13	UFT	O4-C4	-2.90	1.18	1.24
1	A	62	UFT	O4-C4	-2.90	1.18	1.24
1	A	80	UFT	O4-C4	-2.90	1.18	1.24
1	B	92	UFT	O4-C4	-2.90	1.18	1.24
1	B	293	UFT	O4-C4	-2.90	1.18	1.24
1	A	437	UFT	O4-C4	-2.90	1.18	1.24
1	B	609	UFT	O4-C4	-2.90	1.18	1.24
1	B	703	UFT	O4-C4	-2.90	1.18	1.24
1	B	114	CFZ	C2'-C1'	-2.90	1.49	1.53
1	A	279	CFZ	C2'-C1'	-2.90	1.49	1.53
1	A	493	UFT	O4-C4	-2.90	1.18	1.24
1	B	663	UFT	O4-C4	-2.90	1.18	1.24
1	A	504	UFT	O4-C4	-2.90	1.18	1.24
1	B	653	UFT	O4-C4	-2.90	1.18	1.24
1	B	406	CFZ	C2'-C1'	-2.90	1.49	1.53
1	B	94	UFT	O4-C4	-2.90	1.18	1.24
1	B	105	UFT	O4-C4	-2.90	1.18	1.24
1	A	179	UFT	O4-C4	-2.90	1.18	1.24
1	A	260	UFT	O4-C4	-2.90	1.18	1.24
1	B	708	UFT	O4-C4	-2.90	1.18	1.24
1	A	137	UFT	O4-C4	-2.90	1.18	1.24
1	B	466	UFT	O4-C4	-2.90	1.18	1.24
1	B	502	UFT	O4-C4	-2.90	1.18	1.24
1	B	635	UFT	O4-C4	-2.90	1.18	1.24
1	A	75	CFZ	C2'-C1'	-2.90	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	UFT	O4-C4	-2.89	1.18	1.24
1	A	283	UFT	O4-C4	-2.89	1.18	1.24
1	B	669	UFT	O4-C4	-2.89	1.18	1.24
1	B	719	UFT	O4-C4	-2.89	1.18	1.24
1	B	219	CFZ	C2'-C1'	-2.89	1.49	1.53
1	B	377	UFT	O4-C4	-2.89	1.18	1.24
1	B	659	UFT	O4-C4	-2.89	1.18	1.24
1	A	196	UFT	O4-C4	-2.89	1.18	1.24
1	A	447	UFT	O4-C4	-2.89	1.18	1.24
1	A	502	UFT	O4-C4	-2.89	1.18	1.24
1	B	559	UFT	O4-C4	-2.89	1.18	1.24
1	A	79	CFZ	C2'-C1'	-2.89	1.49	1.53
1	B	369	CFZ	C2'-C1'	-2.89	1.49	1.53
1	B	585	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	600	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	101	UFT	O4-C4	-2.89	1.18	1.24
1	A	174	UFT	O4-C4	-2.89	1.18	1.24
1	B	233	UFT	O4-C4	-2.89	1.18	1.24
1	A	633	UFT	O4-C4	-2.89	1.18	1.24
1	A	19	UFT	O4-C4	-2.89	1.18	1.24
1	A	86	UFT	O4-C4	-2.89	1.18	1.24
1	B	305	UFT	O4-C4	-2.89	1.18	1.24
1	A	405	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	208	UFT	O4-C4	-2.89	1.18	1.24
1	B	696	UFT	O4-C4	-2.89	1.18	1.24
1	A	325	CFZ	C2'-C1'	-2.89	1.49	1.53
1	B	59	UFT	O4-C4	-2.89	1.18	1.24
1	A	170	UFT	O4-C4	-2.89	1.18	1.24
1	B	577	UFT	O4-C4	-2.89	1.18	1.24
1	A	217	UFT	O4-C4	-2.89	1.18	1.24
1	B	73	CFZ	C2'-C1'	-2.89	1.49	1.53
1	B	149	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	366	UFT	O4-C4	-2.89	1.18	1.24
1	A	411	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	92	UFT	O4-C4	-2.89	1.18	1.24
1	B	155	UFT	O4-C4	-2.89	1.18	1.24
1	B	190	UFT	O4-C4	-2.89	1.18	1.24
1	A	347	UFT	O4-C4	-2.89	1.18	1.24
1	B	69	UFT	O4-C4	-2.89	1.18	1.24
1	A	334	UFT	O4-C4	-2.89	1.18	1.24
1	B	366	UFT	O4-C4	-2.89	1.18	1.24
1	B	143	UFT	O4-C4	-2.89	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	UFT	O4-C4	-2.89	1.18	1.24
1	B	329	UFT	O4-C4	-2.89	1.18	1.24
1	B	582	UFT	O4-C4	-2.89	1.18	1.24
1	A	690	UFT	O4-C4	-2.89	1.18	1.24
1	A	354	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	355	CFZ	C2'-C1'	-2.89	1.49	1.53
1	B	88	UFT	O4-C4	-2.89	1.18	1.24
1	A	163	UFT	O4-C4	-2.89	1.18	1.24
1	A	708	UFT	O4-C4	-2.89	1.18	1.24
1	B	266	UFT	O4-C4	-2.89	1.18	1.24
1	B	322	UFT	O4-C4	-2.89	1.18	1.24
1	B	485	UFT	O4-C4	-2.89	1.18	1.24
1	B	618	UFT	O4-C4	-2.89	1.18	1.24
1	A	175	UFT	O4-C4	-2.89	1.18	1.24
1	A	646	UFT	O4-C4	-2.89	1.18	1.24
1	B	89	UFT	O4-C4	-2.89	1.18	1.24
1	A	135	UFT	O4-C4	-2.89	1.18	1.24
1	A	544	UFT	O4-C4	-2.89	1.18	1.24
1	B	704	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	313	UFT	O4-C4	-2.89	1.18	1.24
1	A	402	UFT	O4-C4	-2.89	1.18	1.24
1	A	530	UFT	O4-C4	-2.89	1.18	1.24
1	A	474	CFZ	C2'-C1'	-2.89	1.49	1.53
1	B	608	UFT	O4-C4	-2.89	1.18	1.24
1	B	169	UFT	O4-C4	-2.88	1.18	1.24
1	A	628	UFT	O4-C4	-2.88	1.18	1.24
1	A	139	CFZ	C2'-C1'	-2.88	1.49	1.53
1	A	97	UFT	O4-C4	-2.88	1.18	1.24
1	A	695	UFT	O4-C4	-2.88	1.18	1.24
1	B	151	CFZ	C2'-C1'	-2.88	1.49	1.53
1	A	679	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	545	UFT	O4-C4	-2.88	1.18	1.24
1	A	182	UFT	O4-C4	-2.88	1.18	1.24
1	A	55	UFT	O4-C4	-2.88	1.18	1.24
1	B	493	UFT	O4-C4	-2.88	1.18	1.24
1	A	720	UFT	O4-C4	-2.88	1.18	1.24
1	B	316	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	204	UFT	O4-C4	-2.88	1.18	1.24
1	A	301	UFT	O4-C4	-2.88	1.18	1.24
1	B	456	UFT	O4-C4	-2.88	1.18	1.24
1	B	554	UFT	O4-C4	-2.88	1.18	1.24
1	A	126	UFT	O4-C4	-2.88	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	CFZ	C2'-C1'	-2.88	1.49	1.53
1	A	313	UFT	C2'-C1'	-2.88	1.49	1.53
1	B	313	UFT	O4-C4	-2.88	1.18	1.24
1	A	603	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	141	UFT	O4-C4	-2.88	1.18	1.24
1	B	201	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	579	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	682	CFZ	C2'-C1'	-2.88	1.49	1.53
1	A	592	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	651	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	71	UFT	O4-C4	-2.88	1.18	1.24
1	A	542	UFT	O4-C4	-2.88	1.18	1.24
1	B	555	UFT	O4-C4	-2.88	1.18	1.24
1	B	57	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	160	UFT	O4-C4	-2.88	1.18	1.24
1	A	421	UFT	O4-C4	-2.88	1.18	1.24
1	A	369	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	373	CFZ	C2'-C1'	-2.88	1.49	1.53
1	A	585	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	182	UFT	O4-C4	-2.88	1.18	1.24
1	B	260	UFT	O4-C4	-2.88	1.18	1.24
1	A	359	UFT	O4-C4	-2.88	1.18	1.24
1	A	606	UFT	O4-C4	-2.88	1.18	1.24
1	B	411	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	344	UFT	O4-C4	-2.88	1.18	1.24
1	B	26	CFZ	C2'-C1'	-2.88	1.49	1.53
1	A	201	CFZ	C2'-C1'	-2.88	1.49	1.53
1	A	399	CFZ	C2'-C1'	-2.88	1.49	1.53
1	A	548	CFZ	C2'-C1'	-2.88	1.49	1.53
1	B	208	UFT	O4-C4	-2.88	1.18	1.24
1	A	503	UFT	O4-C4	-2.88	1.18	1.24
1	A	212	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	242	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	667	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	94	UFT	O4-C4	-2.87	1.18	1.24
1	A	636	UFT	O4-C4	-2.87	1.18	1.24
1	B	90	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	219	CFZ	C2'-C1'	-2.87	1.49	1.53
1	B	587	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	34	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	204	UFT	O4-C4	-2.87	1.18	1.24
1	A	361	UFT	O4-C4	-2.87	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	621	UFT	O4-C4	-2.87	1.18	1.24
1	A	110	CFZ	C2'-C1'	-2.87	1.49	1.53
1	B	439	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	60	UFT	O4-C4	-2.87	1.18	1.24
1	B	701	UFT	O4-C4	-2.87	1.18	1.24
1	A	656	UFT	O4-C4	-2.87	1.18	1.24
1	B	600	CFZ	C2'-C1'	-2.87	1.49	1.53
1	B	637	CFZ	C2'-C1'	-2.87	1.49	1.53
1	B	667	CFZ	C2'-C1'	-2.87	1.49	1.53
1	B	481	UFT	O4-C4	-2.86	1.18	1.24
1	A	131	CFZ	C2'-C1'	-2.86	1.49	1.53
1	A	305	UFT	O4-C4	-2.86	1.18	1.24
1	B	424	CFZ	C2'-C1'	-2.86	1.49	1.53
1	B	528	CFZ	C2'-C1'	-2.86	1.49	1.53
1	B	196	UFT	O4-C4	-2.86	1.18	1.24
1	B	19	UFT	O4-C4	-2.86	1.18	1.24
1	B	140	CFZ	C2'-C1'	-2.86	1.49	1.53
1	B	540	CFZ	C2'-C1'	-2.86	1.49	1.53
1	A	25	CFZ	C2'-C1'	-2.86	1.49	1.53
1	B	354	CFZ	C2'-C1'	-2.86	1.49	1.53
1	A	335	CFZ	C2'-C1'	-2.86	1.49	1.53
1	B	679	CFZ	C2'-C1'	-2.86	1.49	1.53
1	A	103	CFZ	C2'-C1'	-2.86	1.49	1.53
1	A	353	CFZ	C2'-C1'	-2.86	1.49	1.53
1	A	564	CFZ	C2'-C1'	-2.86	1.49	1.53
1	B	662	UFT	O4-C4	-2.86	1.18	1.24
1	A	517	CFZ	C2'-C1'	-2.86	1.49	1.53
1	B	279	CFZ	C2'-C1'	-2.86	1.49	1.53
1	A	10	CFZ	C2'-C1'	-2.85	1.49	1.53
1	A	373	CFZ	C2'-C1'	-2.85	1.49	1.53
1	B	639	CFZ	C2'-C1'	-2.85	1.49	1.53
1	B	61	UFT	O4-C4	-2.85	1.19	1.24
1	B	558	CFZ	C2'-C1'	-2.85	1.49	1.53
1	B	245	UFT	O4-C4	-2.85	1.19	1.24
1	A	114	CFZ	C2'-C1'	-2.85	1.49	1.53
1	A	473	CFZ	C2'-C1'	-2.85	1.49	1.53
1	A	13	UFT	O4-C4	-2.85	1.19	1.24
1	A	639	CFZ	C2'-C1'	-2.85	1.49	1.53
1	B	351	CFZ	C2'-C1'	-2.85	1.49	1.53
1	A	151	CFZ	C2'-C1'	-2.85	1.49	1.53
1	A	506	CFZ	C2'-C1'	-2.85	1.49	1.53
1	B	700	CFZ	C2'-C1'	-2.84	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	CFZ	C2'-C1'	-2.84	1.49	1.53
1	A	424	CFZ	C2'-C1'	-2.84	1.49	1.53
1	A	614	CFZ	C2'-C1'	-2.84	1.49	1.53
1	A	140	CFZ	C2'-C1'	-2.84	1.49	1.53
1	B	574	CFZ	C2'-C1'	-2.84	1.49	1.53
1	B	233	UFT	C2'-C1'	-2.84	1.49	1.53
1	A	543	CFZ	C2'-C1'	-2.84	1.49	1.53
1	A	217	UFT	C2'-C1'	-2.84	1.49	1.53
1	B	328	CFZ	C2'-C1'	-2.83	1.49	1.53
1	A	691	CFZ	C2'-C1'	-2.83	1.49	1.53
1	B	381	CFZ	C2'-C1'	-2.83	1.49	1.53
1	B	548	CFZ	C2'-C1'	-2.83	1.49	1.53
1	A	583	CFZ	C2'-C1'	-2.83	1.49	1.53
1	B	298	CFZ	C2'-C1'	-2.83	1.49	1.53
1	B	198	CFZ	C2'-C1'	-2.83	1.49	1.53
1	A	246	CFZ	C2'-C1'	-2.83	1.49	1.53
1	B	536	CFZ	C2'-C1'	-2.83	1.49	1.53
1	B	614	CFZ	C2'-C1'	-2.83	1.49	1.53
1	B	335	CFZ	C2'-C1'	-2.83	1.49	1.53
1	A	491	CFZ	C2'-C1'	-2.83	1.49	1.53
1	B	620	CFZ	C2'-C1'	-2.83	1.49	1.53
1	B	384	CFZ	C2'-C1'	-2.82	1.49	1.53
1	B	8	UFT	C2'-C1'	-2.82	1.49	1.53
1	A	441	CFZ	C2'-C1'	-2.82	1.49	1.53
1	B	657	CFZ	C2'-C1'	-2.82	1.49	1.53
1	B	241	CFZ	C2'-C1'	-2.82	1.49	1.53
1	A	610	CFZ	C2'-C1'	-2.82	1.49	1.53
1	B	67	CFZ	C2'-C1'	-2.82	1.49	1.53
1	B	355	CFZ	C2'-C1'	-2.82	1.49	1.53
1	B	34	CFZ	C2'-C1'	-2.82	1.49	1.53
1	A	90	CFZ	C2'-C1'	-2.82	1.49	1.53
1	B	370	CFZ	C2'-C1'	-2.82	1.49	1.53
1	B	438	CFZ	C2'-C1'	-2.82	1.49	1.53
1	A	540	CFZ	C2'-C1'	-2.81	1.49	1.53
1	B	583	CFZ	C2'-C1'	-2.81	1.49	1.53
1	B	72	CFZ	C2'-C1'	-2.81	1.49	1.53
1	A	444	CFZ	C2'-C1'	-2.81	1.49	1.53
1	A	664	CFZ	C2'-C1'	-2.81	1.49	1.53
1	A	439	CFZ	C2'-C1'	-2.81	1.49	1.53
1	B	323	CFZ	C2'-C1'	-2.81	1.49	1.53
1	B	332	CFZ	C2'-C1'	-2.81	1.49	1.53
1	B	664	CFZ	C2'-C1'	-2.81	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	CFZ	C2'-C1'	-2.81	1.49	1.53
1	B	360	CFZ	C2'-C1'	-2.81	1.49	1.53
1	B	139	CFZ	C2'-C1'	-2.81	1.49	1.53
1	A	308	CFZ	C2'-C1'	-2.81	1.49	1.53
1	B	473	CFZ	C2'-C1'	-2.80	1.49	1.53
1	B	474	CFZ	C2'-C1'	-2.80	1.49	1.53
1	B	325	CFZ	C2'-C1'	-2.80	1.49	1.53
1	A	465	CFZ	C2'-C1'	-2.80	1.49	1.53
1	B	610	CFZ	C2'-C1'	-2.80	1.49	1.53
1	B	63	CFZ	C2'-C1'	-2.80	1.49	1.53
1	A	268	CFZ	C2'-C1'	-2.80	1.49	1.53
1	A	407	CFZ	C2'-C1'	-2.80	1.49	1.53
1	B	212	CFZ	C2'-C1'	-2.80	1.49	1.53
1	A	332	CFZ	C2'-C1'	-2.80	1.49	1.53
1	A	469	CFZ	C2'-C1'	-2.80	1.49	1.53
1	B	506	CFZ	C2'-C1'	-2.80	1.49	1.53
1	A	574	CFZ	C2'-C1'	-2.80	1.49	1.53
1	B	161	CFZ	C2'-C1'	-2.80	1.49	1.53
1	A	579	CFZ	C2'-C1'	-2.80	1.49	1.53
1	A	620	CFZ	C2'-C1'	-2.80	1.49	1.53
1	A	171	CFZ	C2'-C1'	-2.79	1.49	1.53
1	B	440	CFZ	C2'-C1'	-2.79	1.49	1.53
1	B	652	CFZ	C2'-C1'	-2.79	1.49	1.53
1	B	135	UFT	C2'-C1'	-2.79	1.49	1.53
1	A	438	CFZ	C2'-C1'	-2.79	1.49	1.53
1	B	156	CFZ	C2'-C1'	-2.79	1.49	1.53
1	A	652	CFZ	C2'-C1'	-2.79	1.49	1.53
1	A	351	CFZ	C2'-C1'	-2.79	1.49	1.53
1	A	462	CFZ	C2'-C1'	-2.79	1.49	1.53
1	B	592	CFZ	C2'-C1'	-2.79	1.49	1.53
1	A	117	CFZ	C2'-C1'	-2.78	1.49	1.53
1	B	79	CFZ	C2'-C1'	-2.78	1.49	1.53
1	A	651	CFZ	C2'-C1'	-2.78	1.49	1.53
1	B	691	CFZ	C2'-C1'	-2.78	1.49	1.53
1	A	135	UFT	C2'-C1'	-2.78	1.49	1.53
1	B	338	CFZ	C2'-C1'	-2.78	1.49	1.53
1	B	407	CFZ	C2'-C1'	-2.78	1.49	1.53
1	A	232	CFZ	C2'-C1'	-2.78	1.49	1.53
1	B	117	CFZ	C2'-C1'	-2.77	1.49	1.53
1	B	523	CFZ	C2'-C1'	-2.77	1.49	1.53
1	B	543	CFZ	C2'-C1'	-2.77	1.49	1.53
1	B	171	CFZ	C2'-C1'	-2.77	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	486	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	63	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	241	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	404	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	498	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	349	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	536	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	625	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	198	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	156	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	130	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	26	CFZ	C2'-C1'	-2.77	1.49	1.53
1	B	465	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	144	CFZ	C2'-C1'	-2.77	1.49	1.53
1	B	130	CFZ	C2'-C1'	-2.76	1.49	1.53
1	A	254	CFZ	C2'-C1'	-2.76	1.49	1.53
1	B	498	CFZ	C2'-C1'	-2.76	1.49	1.53
1	A	265	UFT	C2'-C1'	-2.76	1.49	1.53
1	A	161	CFZ	C2'-C1'	-2.76	1.49	1.53
1	B	208	UFT	C2'-C1'	-2.76	1.49	1.53
1	B	217	UFT	C2'-C1'	-2.76	1.49	1.53
1	A	604	CFZ	C2'-C1'	-2.76	1.49	1.53
1	A	338	CFZ	C2'-C1'	-2.75	1.49	1.53
1	B	308	CFZ	C2'-C1'	-2.75	1.49	1.53
1	B	469	CFZ	C2'-C1'	-2.75	1.49	1.53
1	B	179	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	440	CFZ	C2'-C1'	-2.75	1.49	1.53
1	A	208	UFT	C2'-C1'	-2.75	1.49	1.53
1	B	265	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	384	CFZ	C2'-C1'	-2.75	1.49	1.53
1	B	120	CFZ	C2'-C1'	-2.74	1.49	1.53
1	B	441	CFZ	C2'-C1'	-2.74	1.49	1.53
1	A	704	CFZ	C2'-C1'	-2.74	1.49	1.53
1	B	604	CFZ	C2'-C1'	-2.74	1.49	1.53
1	A	637	CFZ	C2'-C1'	-2.74	1.49	1.53
1	A	15	CFZ	C2'-C1'	-2.74	1.49	1.53
1	B	502	UFT	C2'-C1'	-2.74	1.49	1.53
1	A	382	CFZ	C2'-C1'	-2.74	1.49	1.53
1	B	353	CFZ	C2'-C1'	-2.73	1.49	1.53
1	B	418	CFZ	C2'-C1'	-2.73	1.49	1.53
1	A	179	UFT	C2'-C1'	-2.73	1.49	1.53
1	B	564	CFZ	C2'-C1'	-2.73	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	625	CFZ	C2'-C1'	-2.73	1.49	1.53
1	A	494	CFZ	C2'-C1'	-2.73	1.49	1.53
1	B	283	UFT	C2'-C1'	-2.72	1.49	1.53
1	B	232	CFZ	C2'-C1'	-2.72	1.49	1.53
1	B	268	CFZ	C2'-C1'	-2.72	1.49	1.53
1	A	502	UFT	C2'-C1'	-2.72	1.49	1.53
1	A	418	CFZ	C2'-C1'	-2.72	1.49	1.53
1	B	404	CFZ	C2'-C1'	-2.72	1.49	1.53
1	B	656	UFT	C2'-C1'	-2.72	1.49	1.53
1	A	120	CFZ	C2'-C1'	-2.71	1.49	1.53
1	B	358	UFT	O4-C4	-2.70	1.19	1.24
1	A	535	UFT	C2'-C1'	-2.70	1.49	1.53
1	A	503	UFT	C2'-C1'	-2.70	1.49	1.53
1	A	657	CFZ	C2'-C1'	-2.70	1.49	1.53
1	B	254	CFZ	C2'-C1'	-2.70	1.49	1.53
1	B	15	CFZ	C2'-C1'	-2.69	1.49	1.53
1	B	460	UFT	C2'-C1'	-2.69	1.49	1.53
1	A	283	UFT	C2'-C1'	-2.69	1.49	1.53
1	A	350	UFT	C2'-C1'	-2.69	1.49	1.53
1	A	519	UFT	C2'-C3'	-2.69	1.49	1.52
1	B	485	UFT	C2'-C1'	-2.68	1.49	1.53
1	B	535	UFT	C2'-C1'	-2.68	1.49	1.53
1	B	42	UFT	C2'-C1'	-2.68	1.49	1.53
1	B	493	UFT	O4'-C1'	2.68	1.48	1.42
1	A	460	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	593	UFT	C2'-C1'	-2.67	1.49	1.53
1	B	577	UFT	O4'-C1'	2.67	1.48	1.42
1	B	684	UFT	C2'-C1'	-2.66	1.49	1.53
1	B	491	CFZ	C2'-C1'	-2.66	1.49	1.53
1	A	50	UFT	C2'-C1'	-2.66	1.49	1.53
1	B	358	UFT	O4'-C1'	2.66	1.48	1.42
1	B	293	UFT	C2'-C1'	-2.66	1.49	1.53
1	B	44	UFT	C2'-C1'	-2.66	1.49	1.53
1	B	367	UFT	C2'-C1'	-2.65	1.49	1.53
1	B	204	UFT	C2'-C1'	-2.65	1.49	1.53
1	A	456	UFT	C2'-C1'	-2.65	1.49	1.53
1	A	216	UFT	O4'-C1'	2.65	1.48	1.42
1	A	358	UFT	O4'-C1'	2.65	1.48	1.42
1	B	708	UFT	C2'-C1'	-2.65	1.49	1.53
1	A	519	UFT	O4'-C1'	2.64	1.48	1.42
1	B	329	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	359	UFT	O4'-C1'	2.64	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	524	UFT	O4'-C1'	2.63	1.48	1.42
1	A	204	UFT	C2'-C1'	-2.63	1.49	1.53
1	A	42	UFT	C2'-C1'	-2.63	1.49	1.53
1	B	499	UFT	C2'-C1'	-2.63	1.49	1.53
1	B	720	UFT	O4'-C1'	2.63	1.48	1.42
1	A	108	UFT	C2'-C1'	-2.63	1.49	1.53
1	A	656	UFT	C2'-C1'	-2.63	1.49	1.53
1	A	684	UFT	C2'-C1'	-2.63	1.49	1.53
1	B	42	UFT	O4'-C1'	2.63	1.48	1.42
1	A	11	UFT	C2'-C1'	-2.63	1.49	1.53
1	A	432	UFT	C2'-C1'	-2.63	1.49	1.53
1	B	628	UFT	C2'-C1'	-2.63	1.49	1.53
1	B	43	UFT	C2-N3	2.62	1.42	1.38
1	B	646	UFT	C2'-C1'	-2.62	1.49	1.53
1	B	260	UFT	O4'-C1'	2.62	1.48	1.42
1	B	524	UFT	C2'-C1'	-2.62	1.49	1.53
1	A	216	UFT	C2-N3	2.62	1.42	1.38
1	A	549	UFT	C2'-C1'	-2.62	1.49	1.53
1	B	456	UFT	C2'-C1'	-2.62	1.49	1.53
1	B	602	UFT	C2'-C1'	-2.62	1.49	1.53
1	A	628	UFT	C2'-C1'	-2.62	1.49	1.53
1	A	577	UFT	O4'-C1'	2.61	1.48	1.42
1	B	513	UFT	O4'-C1'	2.61	1.48	1.42
1	B	108	UFT	C2'-C1'	-2.61	1.49	1.53
1	B	432	UFT	O4'-C1'	2.61	1.48	1.42
1	A	530	UFT	O4'-C1'	2.61	1.48	1.42
1	B	430	UFT	C2'-C1'	-2.61	1.49	1.53
1	A	359	UFT	C2-N3	2.61	1.42	1.38
1	B	192	UFT	C2'-C1'	-2.60	1.49	1.53
1	A	80	UFT	O4'-C1'	2.60	1.48	1.42
1	B	13	UFT	C2'-C1'	-2.60	1.49	1.53
1	A	215	UFT	C2-N3	2.60	1.42	1.38
1	B	32	UFT	O4'-C1'	2.60	1.48	1.42
1	A	108	UFT	O4'-C1'	2.60	1.48	1.42
1	A	447	UFT	C2'-C1'	-2.60	1.49	1.53
1	B	216	UFT	O4'-C1'	2.60	1.48	1.42
1	A	629	UFT	O4'-C1'	2.60	1.48	1.42
1	A	322	UFT	O4'-C1'	2.60	1.48	1.42
1	B	629	UFT	O4'-C1'	2.60	1.48	1.42
1	A	84	UFT	C2'-C1'	-2.59	1.49	1.53
1	B	251	UFT	C2'-C1'	-2.59	1.49	1.53
1	B	216	UFT	C2-N3	2.59	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	602	UFT	C2'-C1'	-2.59	1.49	1.53
1	B	669	UFT	C2'-C1'	-2.59	1.49	1.53
1	A	8	UFT	O4'-C1'	2.59	1.48	1.42
1	A	582	UFT	O4'-C1'	2.59	1.48	1.42
1	A	646	UFT	C2'-C1'	-2.59	1.49	1.53
1	A	33	UFT	O4'-C1'	2.59	1.48	1.42
1	A	260	UFT	O4'-C1'	2.59	1.48	1.42
1	B	719	UFT	O4'-C1'	2.59	1.48	1.42
1	B	86	UFT	O4'-C1'	2.59	1.48	1.42
1	A	703	UFT	C2'-C1'	-2.59	1.49	1.53
1	A	535	UFT	O4'-C1'	2.59	1.48	1.42
1	B	493	UFT	C2-N3	2.59	1.42	1.38
1	A	447	UFT	O4'-C1'	2.59	1.48	1.42
1	B	322	UFT	C2'-C1'	-2.59	1.49	1.53
1	A	577	UFT	C2-N3	2.58	1.42	1.38
1	B	606	UFT	C2'-C1'	-2.58	1.49	1.53
1	B	233	UFT	C2-N3	2.58	1.42	1.38
1	B	703	UFT	C2'-C1'	-2.58	1.49	1.53
1	A	175	UFT	C2'-C1'	-2.58	1.49	1.53
1	A	251	UFT	C2'-C1'	-2.58	1.49	1.53
1	A	377	UFT	C2-N3	2.58	1.42	1.38
1	B	301	UFT	C2'-C1'	-2.58	1.49	1.53
1	A	402	UFT	C2'-C1'	-2.58	1.49	1.53
1	B	358	UFT	C2-N3	2.58	1.42	1.38
1	A	344	UFT	C2-N3	2.58	1.42	1.38
1	A	106	UFT	C2'-C1'	-2.58	1.49	1.53
1	A	329	UFT	C2'-C1'	-2.58	1.49	1.53
1	A	8	UFT	C2-N3	2.58	1.42	1.38
1	B	32	UFT	C2-N3	2.58	1.42	1.38
1	B	402	UFT	C2'-C1'	-2.58	1.49	1.53
1	B	673	UFT	C2-N3	2.58	1.42	1.38
1	A	112	UFT	O4'-C1'	2.58	1.48	1.42
1	A	266	UFT	C2'-C1'	-2.58	1.49	1.53
1	B	313	UFT	C2-N3	2.58	1.42	1.38
1	B	112	UFT	C2-N3	2.57	1.42	1.38
1	B	155	UFT	C2-N3	2.57	1.42	1.38
1	A	55	UFT	C2-N3	2.57	1.42	1.38
1	B	377	UFT	C2-N3	2.57	1.42	1.38
1	B	55	UFT	C2-N3	2.57	1.42	1.38
1	A	464	UFT	C2-N3	2.57	1.42	1.38
1	A	571	UFT	C2-N3	2.57	1.42	1.38
1	B	245	UFT	O4'-C1'	2.57	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	UFT	C2'-C1'	-2.57	1.49	1.53
1	A	629	UFT	C2-N3	2.57	1.42	1.38
1	A	432	UFT	O4'-C1'	2.57	1.48	1.42
1	A	509	UFT	C2-N3	2.57	1.42	1.38
1	A	50	UFT	O4'-C1'	2.57	1.48	1.42
1	A	513	UFT	O4'-C1'	2.57	1.48	1.42
1	A	628	UFT	C2-N3	2.57	1.42	1.38
1	A	55	UFT	C2'-C1'	-2.57	1.49	1.53
1	B	535	UFT	O4'-C1'	2.57	1.48	1.42
1	A	361	UFT	C2-N3	2.57	1.42	1.38
1	B	352	UFT	O4'-C1'	2.57	1.48	1.42
1	B	447	UFT	C2'-C1'	-2.57	1.49	1.53
1	A	33	UFT	C2-N3	2.57	1.42	1.38
1	B	398	UFT	C2'-C1'	-2.57	1.49	1.53
1	B	432	UFT	C2'-C1'	-2.57	1.49	1.53
1	B	389	UFT	O4'-C1'	2.57	1.48	1.42
1	A	105	UFT	C2-N3	2.57	1.42	1.38
1	A	571	UFT	C2'-C1'	-2.57	1.49	1.53
1	A	196	UFT	C2-N3	2.57	1.42	1.38
1	A	719	UFT	C2-N3	2.57	1.42	1.38
1	B	80	UFT	C2-N3	2.56	1.42	1.38
1	A	42	UFT	O4'-C1'	2.56	1.48	1.42
1	B	447	UFT	O4'-C1'	2.56	1.48	1.42
1	A	712	UFT	O4'-C1'	2.56	1.48	1.42
1	A	301	UFT	C2-N3	2.56	1.42	1.38
1	B	293	UFT	O4'-C1'	2.56	1.48	1.42
1	B	108	UFT	O4'-C1'	2.56	1.48	1.42
1	A	581	UFT	C2-N3	2.56	1.42	1.38
1	B	689	UFT	C2-N3	2.56	1.42	1.38
1	B	456	UFT	O4'-C1'	2.56	1.48	1.42
1	B	322	UFT	C2-N3	2.56	1.42	1.38
1	A	466	UFT	C2-N3	2.56	1.42	1.38
1	B	33	UFT	O4'-C1'	2.56	1.48	1.42
1	B	430	UFT	C2-N3	2.56	1.42	1.38
1	B	633	UFT	O4'-C1'	2.56	1.48	1.42
1	B	703	UFT	O4'-C1'	2.56	1.48	1.42
1	A	174	UFT	C2-N3	2.56	1.42	1.38
1	B	217	UFT	C2-N3	2.56	1.42	1.38
1	A	502	UFT	C2-N3	2.56	1.42	1.38
1	B	365	UFT	O4'-C1'	2.56	1.48	1.42
1	A	689	UFT	C2-N3	2.56	1.42	1.38
1	B	175	UFT	C2'-C1'	-2.56	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	UFT	C2-N3	2.56	1.42	1.38
1	A	197	UFT	C2-N3	2.56	1.42	1.38
1	A	352	UFT	C2-N3	2.56	1.42	1.38
1	B	153	UFT	C2'-C1'	-2.56	1.49	1.53
1	A	266	UFT	C2-N3	2.56	1.42	1.38
1	B	502	UFT	C2-N3	2.56	1.42	1.38
1	B	519	UFT	C2-N3	2.56	1.42	1.38
1	A	55	UFT	O4'-C1'	2.56	1.48	1.42
1	A	44	UFT	C2'-C1'	-2.56	1.49	1.53
1	B	423	UFT	O4'-C1'	2.56	1.48	1.42
1	B	577	UFT	C2-N3	2.56	1.42	1.38
1	A	486	CFZ	C2'-C1'	-2.56	1.49	1.53
1	B	549	UFT	C2-N3	2.56	1.42	1.38
1	A	358	UFT	C2-N3	2.56	1.42	1.38
1	B	106	UFT	C2'-C1'	-2.56	1.49	1.53
1	A	293	UFT	C2'-C1'	-2.56	1.49	1.53
1	A	545	UFT	C2'-C1'	-2.56	1.49	1.53
1	B	712	UFT	C2'-C1'	-2.56	1.49	1.53
1	B	11	UFT	C2-N3	2.56	1.42	1.38
1	A	50	UFT	C2-N3	2.56	1.42	1.38
1	B	251	UFT	C2-N3	2.56	1.42	1.38
1	A	233	UFT	C2-N3	2.55	1.42	1.38
1	B	266	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	98	UFT	O4'-C1'	2.55	1.48	1.42
1	B	229	UFT	O4'-C1'	2.55	1.48	1.42
1	A	182	UFT	C2-N3	2.55	1.42	1.38
1	A	456	UFT	C2-N3	2.55	1.42	1.38
1	A	636	UFT	C2-N3	2.55	1.42	1.38
1	A	216	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	633	UFT	O4'-C1'	2.55	1.48	1.42
1	B	466	UFT	C2-N3	2.55	1.42	1.38
1	B	137	UFT	C2'-C1'	-2.55	1.49	1.53
1	B	154	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	192	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	554	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	98	UFT	C2-N3	2.55	1.42	1.38
1	A	365	UFT	O4'-C1'	2.55	1.48	1.42
1	B	94	UFT	C2-N3	2.55	1.42	1.38
1	B	636	UFT	C2-N3	2.55	1.42	1.38
1	A	19	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	229	UFT	C2-N3	2.55	1.42	1.38
1	B	403	UFT	C2-N3	2.55	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	UFT	O4'-C1'	2.55	1.48	1.42
1	A	32	UFT	O4'-C1'	2.55	1.48	1.42
1	A	606	UFT	C2-N3	2.55	1.42	1.38
1	A	621	UFT	C2-N3	2.55	1.42	1.38
1	B	628	UFT	C2-N3	2.55	1.42	1.38
1	B	676	UFT	C2-N3	2.55	1.42	1.38
1	A	413	UFT	O4'-C1'	2.55	1.48	1.42
1	A	684	UFT	O4'-C1'	2.55	1.48	1.42
1	B	13	UFT	C2-N3	2.55	1.42	1.38
1	A	43	UFT	C2-N3	2.55	1.42	1.38
1	B	481	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	606	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	389	UFT	O4'-C1'	2.55	1.48	1.42
1	B	687	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	695	UFT	C2'-C1'	-2.55	1.49	1.53
1	B	92	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	86	UFT	O4'-C1'	2.55	1.48	1.42
1	A	204	UFT	O4'-C1'	2.55	1.48	1.42
1	B	98	UFT	O4'-C1'	2.55	1.48	1.42
1	B	112	UFT	O4'-C1'	2.55	1.48	1.42
1	B	69	UFT	C2-N3	2.55	1.42	1.38
1	A	153	UFT	O4'-C1'	2.55	1.48	1.42
1	A	703	UFT	O4'-C1'	2.55	1.48	1.42
1	B	74	UFT	C2-N3	2.55	1.42	1.38
1	A	302	UFT	C2-N3	2.55	1.42	1.38
1	B	534	UFT	C2'-C1'	-2.55	1.49	1.53
1	B	571	UFT	C2'-C1'	-2.55	1.49	1.53
1	A	293	UFT	O4'-C1'	2.55	1.48	1.42
1	B	62	UFT	C2-N3	2.55	1.42	1.38
1	B	559	UFT	C2-N3	2.55	1.42	1.38
1	B	628	UFT	O4'-C1'	2.55	1.48	1.42
1	A	485	UFT	C2-N3	2.55	1.42	1.38
1	B	179	UFT	O4'-C1'	2.54	1.48	1.42
1	B	233	UFT	O4'-C1'	2.54	1.48	1.42
1	B	582	UFT	O4'-C1'	2.54	1.48	1.42
1	B	190	UFT	C2-N3	2.54	1.42	1.38
1	B	500	UFT	C2-N3	2.54	1.42	1.38
1	B	509	UFT	C2-N3	2.54	1.42	1.38
1	A	98	UFT	C2'-C1'	-2.54	1.49	1.53
1	A	489	UFT	C2'-C1'	-2.54	1.49	1.53
1	B	33	UFT	C2-N3	2.54	1.42	1.38
1	A	44	UFT	O4'-C1'	2.54	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	UFT	O4'-C1'	2.54	1.48	1.42
1	A	421	UFT	O4'-C1'	2.54	1.48	1.42
1	B	86	UFT	C2-N3	2.54	1.42	1.38
1	A	112	UFT	C2-N3	2.54	1.42	1.38
1	B	86	UFT	C2'-C1'	-2.54	1.49	1.53
1	A	437	UFT	C2'-C1'	-2.54	1.49	1.53
1	A	712	UFT	C2'-C1'	-2.54	1.49	1.53
1	A	471	UFT	O4'-C1'	2.54	1.48	1.42
1	A	13	UFT	C2-N3	2.54	1.42	1.38
1	A	245	UFT	C2-N3	2.54	1.42	1.38
1	A	687	UFT	O4'-C1'	2.54	1.48	1.42
1	B	84	UFT	C2-N3	2.54	1.42	1.38
1	B	108	UFT	C2-N3	2.54	1.42	1.38
1	A	437	UFT	C2-N3	2.54	1.42	1.38
1	B	116	UFT	C2-N3	2.54	1.42	1.38
1	B	464	UFT	C2-N3	2.54	1.42	1.38
1	A	503	UFT	C2-N3	2.54	1.42	1.38
1	B	265	UFT	C2-N3	2.54	1.42	1.38
1	A	336	UFT	C2-N3	2.54	1.42	1.38
1	B	499	UFT	C2-N3	2.54	1.42	1.38
1	A	456	UFT	O4'-C1'	2.54	1.48	1.42
1	A	135	UFT	C2-N3	2.54	1.42	1.38
1	B	471	UFT	O4'-C1'	2.54	1.48	1.42
1	A	602	UFT	O4'-C1'	2.54	1.48	1.42
1	B	80	UFT	C2'-C1'	-2.54	1.49	1.53
1	A	398	UFT	C2'-C1'	-2.54	1.49	1.53
1	B	208	UFT	C2-N3	2.54	1.42	1.38
1	A	367	UFT	C2'-C1'	-2.54	1.49	1.53
1	B	229	UFT	C2-N3	2.54	1.42	1.38
1	B	431	UFT	C2-N3	2.54	1.42	1.38
1	B	313	UFT	O4'-C1'	2.54	1.48	1.42
1	B	695	UFT	O4'-C1'	2.54	1.48	1.42
1	B	656	UFT	C2-N3	2.54	1.42	1.38
1	A	633	UFT	C2'-C1'	-2.54	1.49	1.53
1	A	155	UFT	O4'-C1'	2.54	1.48	1.42
1	B	434	UFT	C2-N3	2.54	1.42	1.38
1	B	322	UFT	O4'-C1'	2.54	1.48	1.42
1	A	163	UFT	O4'-C1'	2.54	1.48	1.42
1	A	179	UFT	O4'-C1'	2.54	1.48	1.42
1	A	472	UFT	C2-N3	2.54	1.42	1.38
1	A	154	UFT	C2-N3	2.54	1.42	1.38
1	B	581	UFT	C2-N3	2.53	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	UFT	O4'-C1'	2.53	1.48	1.42
1	A	28	CFZ	C2'-C1'	-2.53	1.49	1.53
1	A	153	UFT	C2'-C1'	-2.53	1.49	1.53
1	B	421	UFT	O4'-C1'	2.53	1.48	1.42
1	B	153	UFT	C2-N3	2.53	1.42	1.38
1	A	423	UFT	C2-N3	2.53	1.42	1.38
1	B	708	UFT	C2-N3	2.53	1.42	1.38
1	B	545	UFT	C2'-C1'	-2.53	1.49	1.53
1	A	192	UFT	C2-N3	2.53	1.42	1.38
1	B	361	UFT	C2-N3	2.53	1.42	1.38
1	B	19	UFT	C2-N3	2.53	1.42	1.38
1	A	202	UFT	C2-N3	2.53	1.42	1.38
1	B	204	UFT	C2-N3	2.53	1.42	1.38
1	A	690	UFT	C2-N3	2.53	1.42	1.38
1	A	534	UFT	C2'-C1'	-2.53	1.49	1.53
1	A	169	UFT	C2-N3	2.53	1.42	1.38
1	B	334	UFT	C2-N3	2.53	1.42	1.38
1	B	471	UFT	C2-N3	2.53	1.42	1.38
1	B	695	UFT	C2'-C1'	-2.53	1.49	1.53
1	B	684	UFT	O4'-C1'	2.53	1.48	1.42
1	B	687	UFT	O4'-C1'	2.53	1.48	1.42
1	A	62	UFT	C2-N3	2.53	1.42	1.38
1	A	208	UFT	C2-N3	2.53	1.42	1.38
1	B	344	UFT	C2-N3	2.53	1.42	1.38
1	A	618	UFT	C2-N3	2.53	1.42	1.38
1	A	690	UFT	O4'-C1'	2.53	1.48	1.42
1	B	71	UFT	C2-N3	2.53	1.42	1.38
1	B	105	UFT	C2-N3	2.53	1.42	1.38
1	A	154	UFT	C2'-C1'	-2.53	1.49	1.53
1	B	524	UFT	O4'-C1'	2.53	1.48	1.42
1	B	635	UFT	C2-N3	2.53	1.42	1.38
1	B	309	UFT	O4'-C1'	2.53	1.48	1.42
1	A	106	UFT	C2-N3	2.53	1.42	1.38
1	A	434	UFT	C2-N3	2.53	1.42	1.38
1	B	542	UFT	C2-N3	2.53	1.42	1.38
1	B	367	UFT	C2-N3	2.53	1.42	1.38
1	B	141	UFT	C2-N3	2.53	1.42	1.38
1	A	153	UFT	C2-N3	2.53	1.42	1.38
1	A	260	UFT	C2-N3	2.53	1.42	1.38
1	B	192	UFT	O4'-C1'	2.53	1.48	1.42
1	B	160	UFT	C2-N3	2.53	1.42	1.38
1	B	163	UFT	C2-N3	2.53	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	UFT	C2-N3	2.53	1.42	1.38
1	A	217	UFT	C2-N3	2.53	1.42	1.38
1	A	500	UFT	C2-N3	2.53	1.42	1.38
1	A	607	UFT	C2-N3	2.53	1.42	1.38
1	B	44	UFT	O4'-C1'	2.53	1.48	1.42
1	B	48	UFT	C2-N3	2.53	1.42	1.38
1	B	200	UFT	C2-N3	2.53	1.42	1.38
1	B	283	UFT	C2-N3	2.53	1.42	1.38
1	A	305	UFT	C2-N3	2.53	1.42	1.38
1	B	524	UFT	C2-N3	2.53	1.42	1.38
1	B	602	UFT	C2-N3	2.53	1.42	1.38
1	B	460	UFT	O4'-C1'	2.53	1.48	1.42
1	A	217	UFT	O4'-C1'	2.53	1.48	1.42
1	B	55	UFT	O4'-C1'	2.53	1.48	1.42
1	B	92	UFT	O4'-C1'	2.53	1.48	1.42
1	B	305	UFT	C2-N3	2.53	1.42	1.38
1	A	350	UFT	C2-N3	2.53	1.42	1.38
1	B	60	UFT	C2'-C1'	-2.53	1.49	1.53
1	B	554	UFT	C2'-C1'	-2.53	1.49	1.53
1	A	534	UFT	O4'-C1'	2.53	1.48	1.42
1	B	669	UFT	O4'-C1'	2.53	1.48	1.42
1	A	659	UFT	C2-N3	2.53	1.42	1.38
1	A	720	UFT	C2-N3	2.53	1.42	1.38
1	B	11	UFT	O4'-C1'	2.53	1.48	1.42
1	B	97	UFT	C2'-C1'	-2.53	1.49	1.53
1	B	97	UFT	C2-N3	2.53	1.42	1.38
1	A	163	UFT	C2-N3	2.53	1.42	1.38
1	A	170	UFT	C2-N3	2.53	1.42	1.38
1	B	534	UFT	C2-N3	2.53	1.42	1.38
1	A	460	UFT	O4'-C1'	2.53	1.48	1.42
1	A	549	UFT	C2-N3	2.53	1.42	1.38
1	B	618	UFT	C2-N3	2.53	1.42	1.38
1	B	43	UFT	C2'-C1'	-2.53	1.49	1.53
1	A	669	UFT	C2'-C1'	-2.53	1.49	1.53
1	A	608	UFT	C2-N3	2.52	1.42	1.38
1	B	659	UFT	O4'-C1'	2.52	1.48	1.42
1	B	50	UFT	C2-N3	2.52	1.42	1.38
1	B	266	UFT	O4'-C1'	2.52	1.48	1.42
1	A	59	UFT	O4'-C1'	2.52	1.48	1.42
1	A	329	UFT	C2-N3	2.52	1.42	1.38
1	B	402	UFT	C2-N3	2.52	1.42	1.38
1	A	530	UFT	C2-N3	2.52	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	UFT	C2'-C1'	-2.52	1.49	1.53
1	B	260	UFT	C2'-C1'	-2.52	1.49	1.53
1	B	359	UFT	C2'-C1'	-2.52	1.49	1.53
1	A	628	UFT	O4'-C1'	2.52	1.48	1.42
1	A	92	UFT	C2-N3	2.52	1.42	1.38
1	A	421	UFT	C2-N3	2.52	1.42	1.38
1	A	471	UFT	C2-N3	2.52	1.42	1.38
1	B	629	UFT	C2-N3	2.52	1.42	1.38
1	B	88	UFT	O4'-C1'	2.52	1.48	1.42
1	B	633	UFT	C2'-C1'	-2.52	1.49	1.53
1	A	48	UFT	C2-N3	2.52	1.42	1.38
1	A	89	UFT	C2-N3	2.52	1.42	1.38
1	B	135	UFT	O4'-C1'	2.52	1.48	1.42
1	A	200	UFT	C2'-C1'	-2.52	1.49	1.53
1	B	143	UFT	C2-N3	2.52	1.42	1.38
1	B	302	UFT	C2-N3	2.52	1.42	1.38
1	B	163	UFT	C2'-C1'	-2.52	1.49	1.53
1	A	108	UFT	C2-N3	2.52	1.42	1.38
1	B	154	UFT	C2-N3	2.52	1.42	1.38
1	B	179	UFT	C2-N3	2.52	1.42	1.38
1	B	202	UFT	C2-N3	2.52	1.42	1.38
1	B	663	UFT	C2-N3	2.52	1.42	1.38
1	A	135	UFT	O4'-C1'	2.52	1.48	1.42
1	B	646	UFT	O4'-C1'	2.52	1.48	1.42
1	A	163	UFT	C2'-C1'	-2.52	1.49	1.53
1	A	71	UFT	O4'-C1'	2.52	1.48	1.42
1	A	32	UFT	C2-N3	2.52	1.42	1.38
1	A	499	UFT	C2-N3	2.52	1.42	1.38
1	B	719	UFT	C2-N3	2.52	1.42	1.38
1	B	656	UFT	O4'-C1'	2.52	1.48	1.42
1	B	60	UFT	C2-N3	2.52	1.42	1.38
1	A	71	UFT	C2-N3	2.52	1.42	1.38
1	A	413	UFT	C2-N3	2.52	1.42	1.38
1	A	545	UFT	C2-N3	2.52	1.42	1.38
1	B	214	UFT	O4'-C1'	2.52	1.48	1.42
1	B	712	UFT	O4'-C1'	2.52	1.48	1.42
1	A	155	UFT	C2-N3	2.52	1.42	1.38
1	B	192	UFT	C2-N3	2.52	1.42	1.38
1	B	260	UFT	C2-N3	2.52	1.42	1.38
1	A	653	UFT	O4'-C1'	2.52	1.48	1.42
1	A	142	UFT	C2-N3	2.52	1.42	1.38
1	A	431	UFT	C2-N3	2.52	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	646	UFT	C2-N3	2.52	1.42	1.38
1	A	687	UFT	C2-N3	2.52	1.42	1.38
1	B	80	UFT	O4'-C1'	2.52	1.48	1.42
1	B	367	UFT	O4'-C1'	2.52	1.48	1.42
1	A	8	UFT	C2'-C1'	-2.52	1.49	1.53
1	A	708	UFT	C2'-C1'	-2.52	1.49	1.53
1	B	659	UFT	C2-N3	2.52	1.42	1.38
1	B	509	UFT	O4'-C1'	2.52	1.48	1.42
1	B	137	UFT	O4'-C1'	2.52	1.48	1.42
1	A	676	UFT	O4'-C1'	2.52	1.48	1.42
1	B	170	UFT	C2-N3	2.52	1.42	1.38
1	B	662	UFT	C2-N3	2.52	1.42	1.38
1	A	313	UFT	O4'-C1'	2.52	1.48	1.42
1	A	430	UFT	C2'-C1'	-2.52	1.49	1.53
1	A	101	UFT	C2-N3	2.52	1.42	1.38
1	B	460	UFT	C2-N3	2.52	1.42	1.38
1	A	656	UFT	C2-N3	2.52	1.42	1.38
1	B	329	UFT	O4'-C1'	2.52	1.48	1.42
1	A	545	UFT	O4'-C1'	2.52	1.48	1.42
1	A	695	UFT	O4'-C1'	2.52	1.48	1.42
1	A	141	UFT	C2-N3	2.52	1.42	1.38
1	A	143	UFT	C2-N3	2.52	1.42	1.38
1	A	296	UFT	C2-N3	2.52	1.42	1.38
1	B	423	UFT	C2-N3	2.52	1.42	1.38
1	B	555	UFT	C2-N3	2.52	1.42	1.38
1	A	361	UFT	C2'-C1'	-2.52	1.49	1.53
1	A	88	UFT	O4'-C1'	2.52	1.48	1.42
1	A	293	UFT	C2-N3	2.52	1.42	1.38
1	B	602	UFT	O4'-C1'	2.51	1.48	1.42
1	A	14	UFT	C2-N3	2.51	1.42	1.38
1	A	534	UFT	C2-N3	2.51	1.42	1.38
1	A	554	UFT	C2-N3	2.51	1.42	1.38
1	A	571	UFT	O4'-C1'	2.51	1.48	1.42
1	A	669	UFT	O4'-C1'	2.51	1.48	1.42
1	B	708	UFT	O4'-C1'	2.51	1.48	1.42
1	A	365	UFT	C2'-C1'	-2.51	1.49	1.53
1	A	61	UFT	C2-N3	2.51	1.42	1.38
1	B	169	UFT	C2-N3	2.51	1.42	1.38
1	A	309	UFT	C2-N3	2.51	1.42	1.38
1	A	712	UFT	C2-N3	2.51	1.42	1.38
1	B	344	UFT	O4'-C1'	2.51	1.48	1.42
1	A	659	UFT	O4'-C1'	2.51	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	UFT	O4'-C1'	2.51	1.48	1.42
1	A	74	UFT	C2-N3	2.51	1.42	1.38
1	A	88	UFT	C2-N3	2.51	1.42	1.38
1	B	669	UFT	C2-N3	2.51	1.42	1.38
1	B	98	UFT	C2'-C1'	-2.51	1.49	1.53
1	B	489	UFT	C2'-C1'	-2.51	1.49	1.53
1	A	251	UFT	O4'-C1'	2.51	1.48	1.42
1	A	423	UFT	O4'-C1'	2.51	1.48	1.42
1	A	720	UFT	C2'-C1'	-2.51	1.49	1.53
1	B	106	UFT	C2-N3	2.51	1.42	1.38
1	B	137	UFT	C2-N3	2.51	1.42	1.38
1	A	322	UFT	C2-N3	2.51	1.42	1.38
1	B	646	UFT	C2-N3	2.51	1.42	1.38
1	B	302	UFT	O4'-C1'	2.51	1.48	1.42
1	A	59	UFT	C2-N3	2.51	1.42	1.38
1	A	504	UFT	C2-N3	2.51	1.42	1.38
1	A	676	UFT	C2-N3	2.51	1.42	1.38
1	A	513	UFT	C2'-C1'	-2.51	1.49	1.53
1	B	43	UFT	O4'-C1'	2.51	1.48	1.42
1	A	464	UFT	O4'-C1'	2.51	1.48	1.42
1	B	101	UFT	C2-N3	2.51	1.42	1.38
1	B	182	UFT	C2-N3	2.51	1.42	1.38
1	B	690	UFT	C2-N3	2.51	1.42	1.38
1	A	229	UFT	O4'-C1'	2.51	1.48	1.42
1	A	350	UFT	O4'-C1'	2.51	1.48	1.42
1	A	460	UFT	C2-N3	2.51	1.42	1.38
1	B	398	UFT	O4'-C1'	2.51	1.47	1.42
1	A	607	UFT	O4'-C1'	2.51	1.47	1.42
1	A	86	UFT	C2-N3	2.51	1.42	1.38
1	B	126	UFT	C2-N3	2.51	1.42	1.38
1	A	204	UFT	C2-N3	2.51	1.42	1.38
1	A	367	UFT	C2-N3	2.51	1.42	1.38
1	B	554	UFT	C2-N3	2.51	1.42	1.38
1	B	590	UFT	C2-N3	2.51	1.42	1.38
1	A	663	UFT	C2-N3	2.51	1.42	1.38
1	B	208	UFT	O4'-C1'	2.51	1.47	1.42
1	A	662	UFT	C2-N3	2.51	1.42	1.38
1	A	344	UFT	C2'-C1'	-2.51	1.49	1.53
1	B	344	UFT	C2'-C1'	-2.51	1.49	1.53
1	A	696	UFT	O4'-C1'	2.51	1.47	1.42
1	B	55	UFT	C2'-C1'	-2.51	1.49	1.53
1	A	687	UFT	C2'-C1'	-2.51	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	666	UFT	O4'-C1'	2.51	1.47	1.42
1	A	666	UFT	C2-N3	2.51	1.42	1.38
1	A	413	UFT	C2'-C1'	-2.51	1.49	1.53
1	B	217	UFT	O4'-C1'	2.51	1.47	1.42
1	B	690	UFT	O4'-C1'	2.51	1.47	1.42
1	B	329	UFT	C2-N3	2.51	1.42	1.38
1	B	607	UFT	C2-N3	2.51	1.42	1.38
1	A	635	UFT	C2-N3	2.51	1.42	1.38
1	A	266	UFT	O4'-C1'	2.51	1.47	1.42
1	B	313	UFT	C2'-C1'	-2.51	1.49	1.53
1	A	659	UFT	C2'-C1'	-2.51	1.49	1.53
1	A	542	UFT	O4'-C1'	2.51	1.47	1.42
1	B	549	UFT	O4'-C1'	2.51	1.47	1.42
1	A	214	UFT	C2-N3	2.51	1.42	1.38
1	B	447	UFT	C2-N3	2.51	1.42	1.38
1	B	559	UFT	O4'-C1'	2.51	1.47	1.42
1	A	481	UFT	C2'-C1'	-2.51	1.49	1.53
1	B	196	UFT	C2-N3	2.51	1.42	1.38
1	A	200	UFT	C2-N3	2.51	1.42	1.38
1	B	245	UFT	C2-N3	2.51	1.42	1.38
1	A	513	UFT	C2-N3	2.51	1.42	1.38
1	B	666	UFT	C2-N3	2.51	1.42	1.38
1	A	367	UFT	O4'-C1'	2.51	1.47	1.42
1	B	309	UFT	C2-N3	2.51	1.42	1.38
1	A	347	UFT	C2-N3	2.51	1.42	1.38
1	A	398	UFT	C2-N3	2.51	1.42	1.38
1	A	403	UFT	C2-N3	2.51	1.42	1.38
1	B	582	UFT	C2-N3	2.51	1.42	1.38
1	B	633	UFT	C2-N3	2.51	1.42	1.38
1	A	214	UFT	O4'-C1'	2.51	1.47	1.42
1	A	19	UFT	C2-N3	2.50	1.42	1.38
1	A	609	UFT	C2-N3	2.50	1.42	1.38
1	A	309	UFT	O4'-C1'	2.50	1.47	1.42
1	B	662	UFT	O4'-C1'	2.50	1.47	1.42
1	B	11	UFT	C2'-C1'	-2.50	1.49	1.53
1	B	423	UFT	C2'-C1'	-2.50	1.49	1.53
1	A	663	UFT	C2'-C1'	-2.50	1.49	1.53
1	A	44	UFT	C2-N3	2.50	1.42	1.38
1	B	270	UFT	C2-N3	2.50	1.42	1.38
1	A	673	UFT	C2-N3	2.50	1.42	1.38
1	A	708	UFT	C2-N3	2.50	1.42	1.38
1	A	301	UFT	C2'-C1'	-2.50	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	701	UFT	O4'-C1'	2.50	1.47	1.42
1	A	11	UFT	O4'-C1'	2.50	1.47	1.42
1	A	43	UFT	O4'-C1'	2.50	1.47	1.42
1	A	493	UFT	C2-N3	2.50	1.42	1.38
1	A	653	UFT	C2-N3	2.50	1.42	1.38
1	B	251	UFT	O4'-C1'	2.50	1.47	1.42
1	B	519	UFT	C2'-C1'	-2.50	1.49	1.53
1	B	701	UFT	C2-N3	2.50	1.42	1.38
1	A	179	UFT	C2-N3	2.50	1.42	1.38
1	B	712	UFT	C2-N3	2.50	1.42	1.38
1	A	92	UFT	O4'-C1'	2.50	1.47	1.42
1	A	141	UFT	O4'-C1'	2.50	1.47	1.42
1	A	251	UFT	C2-N3	2.50	1.42	1.38
1	A	313	UFT	C2-N3	2.50	1.42	1.38
1	B	456	UFT	C2-N3	2.50	1.42	1.38
1	B	204	UFT	O4'-C1'	2.50	1.47	1.42
1	B	542	UFT	O4'-C1'	2.50	1.47	1.42
1	A	334	UFT	C2-N3	2.50	1.42	1.38
1	A	593	UFT	C2-N3	2.50	1.42	1.38
1	A	208	UFT	O4'-C1'	2.50	1.47	1.42
1	A	283	UFT	O4'-C1'	2.50	1.47	1.42
1	B	676	UFT	O4'-C1'	2.50	1.47	1.42
1	B	293	UFT	C2-N3	2.50	1.42	1.38
1	A	590	UFT	C2-N3	2.50	1.42	1.38
1	A	302	UFT	C2'-C1'	-2.50	1.49	1.53
1	A	607	UFT	C2'-C1'	-2.50	1.49	1.53
1	B	689	UFT	C2'-C1'	-2.50	1.49	1.53
1	A	485	UFT	O4'-C1'	2.50	1.47	1.42
1	A	504	UFT	O4'-C1'	2.50	1.47	1.42
1	A	708	UFT	O4'-C1'	2.50	1.47	1.42
1	B	175	UFT	C2-N3	2.50	1.42	1.38
1	B	545	UFT	C2-N3	2.50	1.42	1.38
1	A	602	UFT	C2-N3	2.50	1.42	1.38
1	B	163	UFT	O4'-C1'	2.50	1.47	1.42
1	B	377	UFT	O4'-C1'	2.50	1.47	1.42
1	A	430	UFT	O4'-C1'	2.50	1.47	1.42
1	A	489	UFT	C2-N3	2.50	1.42	1.38
1	B	513	UFT	C2-N3	2.50	1.42	1.38
1	B	266	UFT	C2-N3	2.50	1.42	1.38
1	B	621	UFT	C2-N3	2.50	1.42	1.38
1	A	60	UFT	C2'-C1'	-2.50	1.49	1.53
1	B	464	UFT	C2'-C1'	-2.50	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	UFT	C2-N3	2.50	1.42	1.38
1	B	112	UFT	C2'-C1'	-2.50	1.49	1.53
1	A	229	UFT	C2'-C1'	-2.50	1.49	1.53
1	B	265	UFT	O4'-C1'	2.50	1.47	1.42
1	A	402	UFT	O4'-C1'	2.50	1.47	1.42
1	B	530	UFT	O4'-C1'	2.50	1.47	1.42
1	B	534	UFT	O4'-C1'	2.50	1.47	1.42
1	A	60	UFT	C2-N3	2.50	1.42	1.38
1	B	421	UFT	C2-N3	2.50	1.42	1.38
1	A	524	UFT	C2-N3	2.50	1.42	1.38
1	B	402	UFT	O4'-C1'	2.50	1.47	1.42
1	A	270	UFT	C2-N3	2.50	1.42	1.38
1	B	359	UFT	C2-N3	2.50	1.42	1.38
1	B	607	UFT	C2'-C1'	-2.50	1.49	1.53
1	B	499	UFT	O4'-C1'	2.50	1.47	1.42
1	B	88	UFT	C2-N3	2.50	1.42	1.38
1	A	94	UFT	C2-N3	2.50	1.42	1.38
1	A	403	UFT	O4'-C1'	2.50	1.47	1.42
1	B	696	UFT	O4'-C1'	2.50	1.47	1.42
1	B	33	UFT	C2'-C1'	-2.50	1.49	1.53
1	A	112	UFT	C2'-C1'	-2.50	1.49	1.53
1	A	347	UFT	O4'-C1'	2.49	1.47	1.42
1	A	389	UFT	C2-N3	2.49	1.42	1.38
1	B	504	UFT	C2-N3	2.49	1.42	1.38
1	A	684	UFT	C2-N3	2.49	1.42	1.38
1	A	14	UFT	C2'-C1'	-2.49	1.49	1.53
1	A	42	UFT	C2-N3	2.49	1.42	1.38
1	B	366	UFT	C2-N3	2.49	1.42	1.38
1	B	571	UFT	C2-N3	2.49	1.42	1.38
1	B	608	UFT	C2-N3	2.49	1.42	1.38
1	A	69	UFT	C2-N3	2.49	1.42	1.38
1	B	606	UFT	C2-N3	2.49	1.42	1.38
1	A	14	UFT	O4'-C1'	2.49	1.47	1.42
1	A	192	UFT	O4'-C1'	2.49	1.47	1.42
1	A	265	UFT	O4'-C1'	2.49	1.47	1.42
1	B	336	UFT	O4'-C1'	2.49	1.47	1.42
1	B	504	UFT	O4'-C1'	2.49	1.47	1.42
1	B	519	UFT	O4'-C1'	2.49	1.47	1.42
1	A	549	UFT	O4'-C1'	2.49	1.47	1.42
1	A	377	UFT	O4'-C1'	2.49	1.47	1.42
1	A	365	UFT	C2-N3	2.49	1.42	1.38
1	A	366	UFT	C2-N3	2.49	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	437	UFT	C2-N3	2.49	1.42	1.38
1	A	701	UFT	C2-N3	2.49	1.42	1.38
1	B	141	UFT	O4'-C1'	2.49	1.47	1.42
1	B	359	UFT	O4'-C1'	2.49	1.47	1.42
1	A	656	UFT	O4'-C1'	2.49	1.47	1.42
1	A	190	UFT	C2-N3	2.49	1.42	1.38
1	A	402	UFT	C2-N3	2.49	1.42	1.38
1	A	519	UFT	C2-N3	2.49	1.42	1.38
1	A	542	UFT	C2-N3	2.49	1.42	1.38
1	B	71	UFT	O4'-C1'	2.49	1.47	1.42
1	A	197	UFT	O4'-C1'	2.49	1.47	1.42
1	A	245	UFT	O4'-C1'	2.49	1.47	1.42
1	A	398	UFT	O4'-C1'	2.49	1.47	1.42
1	A	559	UFT	C2-N3	2.49	1.42	1.38
1	A	509	UFT	O4'-C1'	2.49	1.47	1.42
1	B	653	UFT	O4'-C1'	2.49	1.47	1.42
1	B	689	UFT	O4'-C1'	2.49	1.47	1.42
1	B	389	UFT	C2-N3	2.49	1.42	1.38
1	B	155	UFT	O4'-C1'	2.49	1.47	1.42
1	B	684	UFT	C2-N3	2.49	1.42	1.38
1	B	61	UFT	C2'-C1'	-2.49	1.49	1.53
1	A	116	UFT	C2'-C1'	-2.49	1.49	1.53
1	A	190	UFT	C2'-C1'	-2.49	1.49	1.53
1	A	666	UFT	O4'-C1'	2.49	1.47	1.42
1	B	485	UFT	C2-N3	2.49	1.42	1.38
1	B	14	UFT	C2'-C1'	-2.49	1.49	1.53
1	B	635	UFT	C2'-C1'	-2.49	1.49	1.53
1	A	215	UFT	O4'-C1'	2.49	1.47	1.42
1	B	464	UFT	O4'-C1'	2.49	1.47	1.42
1	B	115	UFT	C2-N3	2.49	1.42	1.38
1	B	296	UFT	C2-N3	2.49	1.42	1.38
1	B	434	UFT	O4'-C1'	2.49	1.47	1.42
1	A	80	UFT	C2-N3	2.49	1.42	1.38
1	A	669	UFT	C2-N3	2.49	1.42	1.38
1	B	61	UFT	C2-N3	2.49	1.42	1.38
1	B	135	UFT	C2-N3	2.49	1.42	1.38
1	A	71	UFT	C2'-C1'	-2.49	1.49	1.53
1	B	653	UFT	C2-N3	2.49	1.42	1.38
1	B	196	UFT	O4'-C1'	2.49	1.47	1.42
1	A	233	UFT	C2'-C1'	-2.49	1.49	1.53
1	A	555	UFT	C2-N3	2.49	1.42	1.38
1	B	695	UFT	C2-N3	2.49	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	696	UFT	C2-N3	2.49	1.42	1.38
1	A	432	UFT	C2-N3	2.49	1.42	1.38
1	B	535	UFT	C2-N3	2.49	1.42	1.38
1	A	633	UFT	C2-N3	2.49	1.42	1.38
1	A	582	UFT	C2-N3	2.49	1.42	1.38
1	A	175	UFT	C2-N3	2.48	1.42	1.38
1	A	137	UFT	O4'-C1'	2.48	1.47	1.42
1	A	493	UFT	C2'-C1'	-2.48	1.49	1.53
1	B	98	UFT	C2-N3	2.48	1.42	1.38
1	A	137	UFT	C2-N3	2.48	1.42	1.38
1	B	215	UFT	C2-N3	2.48	1.42	1.38
1	B	14	UFT	O4'-C1'	2.48	1.47	1.42
1	A	554	UFT	O4'-C1'	2.48	1.47	1.42
1	B	365	UFT	C2'-C1'	-2.48	1.49	1.53
1	B	92	UFT	C2-N3	2.48	1.42	1.38
1	A	116	UFT	C2-N3	2.48	1.42	1.38
1	B	544	UFT	C2-N3	2.48	1.42	1.38
1	B	175	UFT	O4'-C1'	2.48	1.47	1.42
1	A	265	UFT	C2-N3	2.48	1.42	1.38
1	B	593	UFT	C2-N3	2.48	1.42	1.38
1	B	202	UFT	O4'-C1'	2.48	1.47	1.42
1	B	42	UFT	C2-N3	2.48	1.42	1.38
1	B	89	UFT	C2-N3	2.48	1.42	1.38
1	B	609	UFT	C2-N3	2.48	1.42	1.38
1	A	695	UFT	C2-N3	2.48	1.42	1.38
1	B	509	UFT	C2'-C1'	-2.48	1.49	1.53
1	A	524	UFT	C2'-C1'	-2.48	1.49	1.53
1	B	214	UFT	C2-N3	2.48	1.42	1.38
1	B	215	UFT	O4'-C1'	2.48	1.47	1.42
1	B	403	UFT	O4'-C1'	2.48	1.47	1.42
1	B	74	UFT	C2'-C1'	-2.48	1.49	1.53
1	B	61	UFT	O4'-C1'	2.48	1.47	1.42
1	B	530	UFT	C2-N3	2.48	1.42	1.38
1	B	421	UFT	C2'-C1'	-2.48	1.49	1.53
1	B	283	UFT	O4'-C1'	2.48	1.47	1.42
1	A	646	UFT	O4'-C1'	2.48	1.47	1.42
1	B	336	UFT	C2-N3	2.48	1.42	1.38
1	B	472	UFT	C2-N3	2.48	1.42	1.38
1	A	653	UFT	C2'-C1'	-2.48	1.49	1.53
1	A	160	UFT	C2-N3	2.48	1.42	1.38
1	A	233	UFT	O4'-C1'	2.48	1.47	1.42
1	B	143	UFT	C2'-C1'	-2.48	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	UFT	C2'-C1'	-2.48	1.49	1.53
1	B	430	UFT	O4'-C1'	2.48	1.47	1.42
1	B	8	UFT	C2-N3	2.48	1.42	1.38
1	A	336	UFT	O4'-C1'	2.48	1.47	1.42
1	B	571	UFT	O4'-C1'	2.48	1.47	1.42
1	B	347	UFT	C2'-C1'	-2.48	1.49	1.53
1	A	544	UFT	C2'-C1'	-2.48	1.49	1.53
1	B	719	UFT	C2'-C1'	-2.48	1.49	1.53
1	A	352	UFT	O4'-C1'	2.48	1.47	1.42
1	A	593	UFT	O4'-C1'	2.48	1.47	1.42
1	B	687	UFT	C2-N3	2.48	1.42	1.38
1	A	296	UFT	O4'-C1'	2.48	1.47	1.42
1	A	559	UFT	O4'-C1'	2.48	1.47	1.42
1	A	703	UFT	C2-N3	2.48	1.42	1.38
1	A	662	UFT	O4'-C1'	2.48	1.47	1.42
1	B	197	UFT	C2-N3	2.48	1.42	1.38
1	A	137	UFT	C2'-C1'	-2.48	1.49	1.53
1	A	283	UFT	C2-N3	2.48	1.42	1.38
1	A	84	UFT	C2-N3	2.47	1.42	1.38
1	B	97	UFT	O4'-C1'	2.47	1.47	1.42
1	B	190	UFT	O4'-C1'	2.47	1.47	1.42
1	A	481	UFT	C2-N3	2.47	1.42	1.38
1	A	101	UFT	C2'-C1'	-2.47	1.49	1.53
1	A	260	UFT	C2'-C1'	-2.47	1.49	1.53
1	B	13	UFT	O4'-C1'	2.47	1.47	1.42
1	B	701	UFT	O4'-C1'	2.47	1.47	1.42
1	A	97	UFT	C2-N3	2.47	1.42	1.38
1	B	398	UFT	C2-N3	2.47	1.42	1.38
1	B	481	UFT	C2-N3	2.47	1.42	1.38
1	A	169	UFT	O4'-C1'	2.47	1.47	1.42
1	A	503	UFT	O4'-C1'	2.47	1.47	1.42
1	A	421	UFT	C2'-C1'	-2.47	1.49	1.53
1	A	635	UFT	O4'-C1'	2.47	1.47	1.42
1	A	175	UFT	O4'-C1'	2.47	1.47	1.42
1	A	215	UFT	C2'-C1'	-2.47	1.49	1.53
1	A	696	UFT	C2-N3	2.47	1.42	1.38
1	B	106	UFT	O4'-C1'	2.47	1.47	1.42
1	B	545	UFT	O4'-C1'	2.47	1.47	1.42
1	B	437	UFT	O4'-C1'	2.47	1.47	1.42
1	B	200	UFT	C2'-C1'	-2.47	1.49	1.53
1	A	544	UFT	C2-N3	2.47	1.42	1.38
1	B	229	UFT	C2'-C1'	-2.47	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	UFT	C2'-C1'	-2.47	1.49	1.53
1	A	485	UFT	C2'-C1'	-2.47	1.49	1.53
1	A	19	UFT	O4'-C1'	2.47	1.47	1.42
1	B	366	UFT	O4'-C1'	2.47	1.47	1.42
1	A	437	UFT	O4'-C1'	2.47	1.47	1.42
1	A	481	UFT	O4'-C1'	2.47	1.47	1.42
1	B	301	UFT	C2-N3	2.47	1.42	1.38
1	A	366	UFT	O4'-C1'	2.47	1.47	1.42
1	A	86	UFT	C2'-C1'	-2.47	1.49	1.53
1	B	302	UFT	C2'-C1'	-2.47	1.49	1.53
1	B	663	UFT	C2'-C1'	-2.47	1.49	1.53
1	B	347	UFT	C2-N3	2.47	1.42	1.38
1	A	174	UFT	O4'-C1'	2.47	1.47	1.42
1	B	703	UFT	C2-N3	2.47	1.42	1.38
1	B	19	UFT	C2'-C1'	-2.47	1.49	1.53
1	A	673	UFT	O4'-C1'	2.47	1.47	1.42
1	B	635	UFT	O4'-C1'	2.47	1.47	1.42
1	A	689	UFT	C2'-C1'	-2.47	1.49	1.53
1	B	44	UFT	C2-N3	2.47	1.42	1.38
1	A	115	UFT	C2-N3	2.47	1.42	1.38
1	A	142	UFT	C2'-C1'	-2.47	1.49	1.53
1	B	101	UFT	O4'-C1'	2.47	1.47	1.42
1	B	84	UFT	O4'-C1'	2.46	1.47	1.42
1	B	544	UFT	C2'-C1'	-2.46	1.49	1.53
1	A	160	UFT	O4'-C1'	2.46	1.47	1.42
1	B	361	UFT	O4'-C1'	2.46	1.47	1.42
1	A	11	UFT	C2-N3	2.46	1.42	1.38
1	A	464	UFT	C2'-C1'	-2.46	1.49	1.53
1	B	94	UFT	O4'-C1'	2.46	1.47	1.42
1	A	430	UFT	C2-N3	2.46	1.42	1.38
1	B	500	UFT	O4'-C1'	2.46	1.47	1.42
1	A	581	UFT	O4'-C1'	2.46	1.47	1.42
1	B	142	UFT	O4'-C1'	2.46	1.47	1.42
1	B	169	UFT	O4'-C1'	2.46	1.47	1.42
1	A	582	UFT	C2'-C1'	-2.46	1.49	1.53
1	B	365	UFT	C2-N3	2.46	1.42	1.38
1	A	115	UFT	C2'-C1'	-2.46	1.49	1.53
1	B	431	UFT	C2'-C1'	-2.46	1.49	1.53
1	A	606	UFT	O4'-C1'	2.46	1.47	1.42
1	B	160	UFT	O4'-C1'	2.46	1.47	1.42
1	B	116	UFT	C2'-C1'	-2.46	1.49	1.53
1	A	169	UFT	C2'-C1'	-2.46	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	UFT	C2'-C1'	-2.46	1.49	1.53
1	B	89	UFT	O4'-C1'	2.46	1.47	1.42
1	B	296	UFT	O4'-C1'	2.46	1.47	1.42
1	B	69	UFT	C2'-C1'	-2.46	1.49	1.53
1	A	126	UFT	C2-N3	2.46	1.42	1.38
1	A	105	UFT	O4'-C1'	2.46	1.47	1.42
1	A	106	UFT	O4'-C1'	2.46	1.47	1.42
1	A	196	UFT	O4'-C1'	2.46	1.47	1.42
1	A	720	UFT	O4'-C1'	2.46	1.47	1.42
1	B	71	UFT	C2'-C1'	-2.46	1.49	1.53
1	B	471	UFT	C2'-C1'	-2.46	1.49	1.53
1	B	59	UFT	C2-N3	2.45	1.42	1.38
1	A	389	UFT	C2'-C1'	-2.45	1.49	1.53
1	A	434	UFT	O4'-C1'	2.45	1.47	1.42
1	A	689	UFT	O4'-C1'	2.45	1.47	1.42
1	B	581	UFT	O4'-C1'	2.45	1.47	1.42
1	B	8	UFT	O4'-C1'	2.45	1.47	1.42
1	A	142	UFT	O4'-C1'	2.45	1.47	1.42
1	B	659	UFT	C2'-C1'	-2.45	1.49	1.53
1	B	116	UFT	O4'-C1'	2.45	1.47	1.42
1	A	431	UFT	O4'-C1'	2.45	1.47	1.42
1	B	720	UFT	C2-N3	2.45	1.42	1.38
1	B	115	UFT	O4'-C1'	2.45	1.47	1.42
1	A	88	UFT	C2'-C1'	-2.45	1.49	1.53
1	A	431	UFT	C2'-C1'	-2.45	1.49	1.53
1	B	352	UFT	C2-N3	2.45	1.42	1.38
1	A	334	UFT	O4'-C1'	2.45	1.47	1.42
1	A	690	UFT	C2'-C1'	-2.45	1.49	1.53
1	B	214	UFT	C2'-C1'	-2.45	1.49	1.53
1	B	48	UFT	C2'-C1'	-2.45	1.49	1.53
1	A	471	UFT	C2'-C1'	-2.45	1.49	1.53
1	B	590	UFT	C2'-C1'	-2.45	1.49	1.53
1	A	636	UFT	C2'-C1'	-2.45	1.49	1.53
1	B	69	UFT	O4'-C1'	2.45	1.47	1.42
1	B	629	UFT	C2'-C1'	-2.45	1.49	1.53
1	B	142	UFT	C2-N3	2.45	1.42	1.38
1	B	466	UFT	O4'-C1'	2.45	1.47	1.42
1	B	190	UFT	C2'-C1'	-2.45	1.49	1.53
1	B	174	UFT	O4'-C1'	2.44	1.47	1.42
1	A	609	UFT	O4'-C1'	2.44	1.47	1.42
1	B	690	UFT	C2'-C1'	-2.44	1.49	1.53
1	B	334	UFT	O4'-C1'	2.44	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	UFT	O4'-C1'	2.44	1.47	1.42
1	B	169	UFT	C2'-C1'	-2.44	1.49	1.53
1	A	377	UFT	C2'-C1'	-2.44	1.49	1.53
1	A	621	UFT	C2'-C1'	-2.44	1.49	1.53
1	B	60	UFT	O4'-C1'	2.44	1.47	1.42
1	A	94	UFT	O4'-C1'	2.44	1.47	1.42
1	A	636	UFT	O4'-C1'	2.44	1.47	1.42
1	B	489	UFT	C2-N3	2.44	1.42	1.38
1	A	59	UFT	C2'-C1'	-2.44	1.49	1.53
1	B	542	UFT	C2'-C1'	-2.44	1.49	1.53
1	B	105	UFT	O4'-C1'	2.44	1.47	1.42
1	A	296	UFT	C2'-C1'	-2.44	1.49	1.53
1	B	352	UFT	C2'-C1'	-2.44	1.49	1.53
1	A	472	UFT	O4'-C1'	2.44	1.47	1.42
1	A	629	UFT	C2'-C1'	-2.44	1.49	1.53
1	B	696	UFT	C2'-C1'	-2.44	1.49	1.53
1	A	101	UFT	O4'-C1'	2.44	1.47	1.42
1	A	143	UFT	C2'-C1'	-2.44	1.49	1.53
1	A	509	UFT	C2'-C1'	-2.44	1.49	1.53
1	A	701	UFT	C2'-C1'	-2.44	1.49	1.53
1	A	245	UFT	C2'-C1'	-2.44	1.49	1.53
1	A	61	UFT	O4'-C1'	2.44	1.47	1.42
1	B	154	UFT	O4'-C1'	2.44	1.47	1.42
1	B	606	UFT	O4'-C1'	2.44	1.47	1.42
1	A	662	UFT	C2'-C1'	-2.44	1.49	1.53
1	B	607	UFT	O4'-C1'	2.44	1.47	1.42
1	B	200	UFT	O4'-C1'	2.44	1.47	1.42
1	B	554	UFT	O4'-C1'	2.44	1.47	1.42
1	A	544	UFT	O4'-C1'	2.43	1.47	1.42
1	B	432	UFT	C2-N3	2.43	1.42	1.38
1	A	170	UFT	C2'-C1'	-2.43	1.49	1.53
1	A	270	UFT	C2'-C1'	-2.43	1.49	1.53
1	A	466	UFT	O4'-C1'	2.43	1.47	1.42
1	B	50	UFT	O4'-C1'	2.43	1.47	1.42
1	B	59	UFT	O4'-C1'	2.43	1.47	1.42
1	A	69	UFT	O4'-C1'	2.43	1.47	1.42
1	B	197	UFT	O4'-C1'	2.43	1.47	1.42
1	B	62	UFT	C2'-C1'	-2.43	1.49	1.53
1	B	662	UFT	C2'-C1'	-2.43	1.49	1.53
1	B	437	UFT	C2'-C1'	-2.43	1.49	1.53
1	A	542	UFT	C2'-C1'	-2.43	1.49	1.53
1	B	115	UFT	C2'-C1'	-2.43	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	UFT	C2'-C1'	-2.43	1.49	1.53
1	B	309	UFT	C2'-C1'	-2.43	1.49	1.53
1	A	322	UFT	C2'-C1'	-2.43	1.49	1.53
1	A	344	UFT	O4'-C1'	2.43	1.47	1.42
1	B	481	UFT	O4'-C1'	2.43	1.47	1.42
1	A	115	UFT	O4'-C1'	2.43	1.47	1.42
1	B	513	UFT	C2'-C1'	-2.43	1.49	1.53
1	B	502	UFT	O4'-C1'	2.43	1.47	1.42
1	B	88	UFT	C2'-C1'	-2.43	1.49	1.53
1	A	60	UFT	O4'-C1'	2.43	1.47	1.42
1	A	423	UFT	C2'-C1'	-2.43	1.49	1.53
1	B	530	UFT	C2'-C1'	-2.43	1.49	1.53
1	A	577	UFT	C2'-C1'	-2.43	1.49	1.53
1	B	609	UFT	O4'-C1'	2.43	1.47	1.42
1	A	126	UFT	O4'-C1'	2.43	1.47	1.42
1	B	489	UFT	O4'-C1'	2.43	1.47	1.42
1	A	719	UFT	O4'-C1'	2.43	1.47	1.42
1	B	609	UFT	C2'-C1'	-2.43	1.49	1.53
1	B	608	UFT	C2'-C1'	-2.43	1.49	1.53
1	B	618	UFT	O4'-C1'	2.42	1.47	1.42
1	B	666	UFT	C2'-C1'	-2.42	1.49	1.53
1	B	431	UFT	O4'-C1'	2.42	1.47	1.42
1	A	33	UFT	C2'-C1'	-2.42	1.49	1.53
1	B	577	UFT	C2'-C1'	-2.42	1.49	1.53
1	A	696	UFT	C2'-C1'	-2.42	1.49	1.53
1	A	535	UFT	C2-N3	2.42	1.42	1.38
1	A	154	UFT	O4'-C1'	2.42	1.47	1.42
1	A	170	UFT	O4'-C1'	2.42	1.47	1.42
1	B	142	UFT	C2'-C1'	-2.42	1.49	1.53
1	A	80	UFT	C2'-C1'	-2.42	1.49	1.53
1	A	618	UFT	O4'-C1'	2.42	1.47	1.42
1	B	673	UFT	O4'-C1'	2.42	1.47	1.42
1	A	673	UFT	C2'-C1'	-2.42	1.49	1.53
1	A	608	UFT	O4'-C1'	2.42	1.47	1.42
1	B	62	UFT	O4'-C1'	2.42	1.47	1.42
1	B	19	UFT	O4'-C1'	2.42	1.47	1.42
1	B	621	UFT	O4'-C1'	2.42	1.47	1.42
1	A	190	UFT	O4'-C1'	2.42	1.47	1.42
1	B	636	UFT	O4'-C1'	2.42	1.47	1.42
1	A	97	UFT	C2'-C1'	-2.42	1.49	1.53
1	A	499	UFT	C2'-C1'	-2.42	1.49	1.53
1	B	590	UFT	O4'-C1'	2.42	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	UFT	C2'-C1'	-2.41	1.49	1.53
1	B	270	UFT	O4'-C1'	2.41	1.47	1.42
1	A	202	UFT	O4'-C1'	2.41	1.47	1.42
1	B	160	UFT	C2'-C1'	-2.41	1.49	1.53
1	A	504	UFT	C2'-C1'	-2.41	1.49	1.53
1	A	200	UFT	O4'-C1'	2.41	1.47	1.42
1	A	61	UFT	C2'-C1'	-2.41	1.49	1.53
1	A	270	UFT	O4'-C1'	2.41	1.47	1.42
1	B	182	UFT	O4'-C1'	2.41	1.47	1.42
1	B	334	UFT	C2'-C1'	-2.41	1.49	1.53
1	B	500	UFT	C2'-C1'	-2.41	1.49	1.53
1	A	555	UFT	C2'-C1'	-2.41	1.49	1.53
1	B	126	UFT	C2'-C1'	-2.41	1.49	1.53
1	A	116	UFT	O4'-C1'	2.41	1.47	1.42
1	A	621	UFT	O4'-C1'	2.41	1.47	1.42
1	A	48	UFT	C2'-C1'	-2.41	1.49	1.53
1	A	62	UFT	O4'-C1'	2.41	1.47	1.42
1	B	544	UFT	O4'-C1'	2.41	1.47	1.42
1	B	636	UFT	C2'-C1'	-2.41	1.49	1.53
1	A	84	UFT	O4'-C1'	2.41	1.47	1.42
1	B	215	UFT	C2'-C1'	-2.41	1.49	1.53
1	A	97	UFT	O4'-C1'	2.41	1.47	1.42
1	A	182	UFT	O4'-C1'	2.41	1.47	1.42
1	B	126	UFT	O4'-C1'	2.41	1.47	1.42
1	B	143	UFT	O4'-C1'	2.41	1.47	1.42
1	B	555	UFT	C2'-C1'	-2.41	1.50	1.53
1	B	653	UFT	C2'-C1'	-2.41	1.50	1.53
1	A	305	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	500	UFT	O4'-C1'	2.40	1.47	1.42
1	B	434	UFT	C2'-C1'	-2.40	1.50	1.53
1	B	581	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	676	UFT	C2'-C1'	-2.40	1.50	1.53
1	B	101	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	309	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	403	UFT	C2'-C1'	-2.40	1.50	1.53
1	B	466	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	502	UFT	O4'-C1'	2.40	1.47	1.42
1	A	74	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	94	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	197	UFT	C2'-C1'	-2.40	1.50	1.53
1	B	377	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	590	UFT	C2'-C1'	-2.40	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	581	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	89	UFT	O4'-C1'	2.39	1.47	1.42
1	A	48	UFT	O4'-C1'	2.39	1.47	1.42
1	A	69	UFT	C2'-C1'	-2.39	1.50	1.53
1	B	559	UFT	C2'-C1'	-2.39	1.50	1.53
1	B	472	UFT	C2'-C1'	-2.39	1.50	1.53
1	A	609	UFT	C2'-C1'	-2.39	1.50	1.53
1	A	366	UFT	C2'-C1'	-2.39	1.50	1.53
1	A	301	UFT	O4'-C1'	2.39	1.47	1.42
1	A	555	UFT	O4'-C1'	2.39	1.47	1.42
1	A	590	UFT	O4'-C1'	2.39	1.47	1.42
1	A	155	UFT	C2'-C1'	-2.39	1.50	1.53
1	A	336	UFT	C2'-C1'	-2.39	1.50	1.53
1	B	403	UFT	C2'-C1'	-2.39	1.50	1.53
1	B	347	UFT	O4'-C1'	2.39	1.47	1.42
1	B	301	UFT	O4'-C1'	2.38	1.47	1.42
1	A	489	UFT	O4'-C1'	2.38	1.47	1.42
1	B	621	UFT	C2'-C1'	-2.38	1.50	1.53
1	B	472	UFT	O4'-C1'	2.38	1.47	1.42
1	B	389	UFT	C2'-C1'	-2.38	1.50	1.53
1	A	434	UFT	C2'-C1'	-2.38	1.50	1.53
1	A	14	UFT	O2-C2	-2.38	1.18	1.23
1	B	89	UFT	C2'-C1'	-2.38	1.50	1.53
1	B	582	UFT	C2'-C1'	-2.38	1.50	1.53
1	B	170	UFT	O4'-C1'	2.38	1.47	1.42
1	A	160	UFT	C2'-C1'	-2.38	1.50	1.53
1	B	94	UFT	C2'-C1'	-2.38	1.50	1.53
1	B	305	UFT	C2'-C1'	-2.38	1.50	1.53
1	B	720	UFT	C2'-C1'	-2.38	1.50	1.53
1	A	666	UFT	C2'-C1'	-2.38	1.50	1.53
1	B	673	UFT	C2'-C1'	-2.38	1.50	1.53
1	A	13	UFT	O4'-C1'	2.37	1.47	1.42
1	B	296	UFT	C2'-C1'	-2.37	1.50	1.53
1	A	466	UFT	C2'-C1'	-2.37	1.50	1.53
1	A	500	UFT	C2'-C1'	-2.37	1.50	1.53
1	A	13	UFT	C2'-C1'	-2.37	1.50	1.53
1	B	197	UFT	C2'-C1'	-2.37	1.50	1.53
1	B	663	UFT	O4'-C1'	2.37	1.47	1.42
1	A	32	UFT	C2'-C1'	-2.37	1.50	1.53
1	A	62	UFT	C2'-C1'	-2.37	1.50	1.53
1	A	126	UFT	C2'-C1'	-2.37	1.50	1.53
1	B	701	UFT	C2'-C1'	-2.37	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	663	UFT	O4'-C1'	2.37	1.47	1.42
1	B	608	UFT	O4'-C1'	2.37	1.47	1.42
1	B	59	UFT	C2'-C1'	-2.37	1.50	1.53
1	B	593	UFT	C2'-C1'	-2.37	1.50	1.53
1	A	89	UFT	C2'-C1'	-2.37	1.50	1.53
1	A	618	UFT	C2'-C1'	-2.37	1.50	1.53
1	B	593	UFT	O4'-C1'	2.36	1.47	1.42
1	A	143	UFT	O4'-C1'	2.36	1.47	1.42
1	A	361	UFT	O4'-C1'	2.36	1.47	1.42
1	B	141	UFT	C2'-C1'	-2.36	1.50	1.53
1	B	170	UFT	C2'-C1'	-2.36	1.50	1.53
1	B	555	UFT	O4'-C1'	2.36	1.47	1.42
1	B	245	UFT	C2'-C1'	-2.36	1.50	1.53
1	B	618	UFT	C2'-C1'	-2.36	1.50	1.53
1	A	608	UFT	C2'-C1'	-2.36	1.50	1.53
1	A	530	UFT	C2'-C1'	-2.36	1.50	1.53
1	A	493	UFT	O4'-C1'	2.36	1.47	1.42
1	B	676	UFT	C2'-C1'	-2.36	1.50	1.53
1	B	74	UFT	O4'-C1'	2.36	1.47	1.42
1	B	485	UFT	O4'-C1'	2.35	1.47	1.42
1	B	366	UFT	C2'-C1'	-2.35	1.50	1.53
1	A	141	UFT	C2'-C1'	-2.35	1.50	1.53
1	B	50	UFT	C2'-C1'	-2.34	1.50	1.53
1	B	155	UFT	C2'-C1'	-2.34	1.50	1.53
1	B	504	UFT	C2'-C1'	-2.34	1.50	1.53
1	B	196	UFT	C2'-C1'	-2.34	1.50	1.53
1	A	74	UFT	O4'-C1'	2.34	1.47	1.42
1	A	202	UFT	C2'-C1'	-2.34	1.50	1.53
1	B	270	UFT	C2'-C1'	-2.34	1.50	1.53
1	B	283	UFT	O2-C2	-2.33	1.18	1.23
1	A	174	UFT	C2'-C1'	-2.33	1.50	1.53
1	A	719	UFT	C2'-C1'	-2.33	1.50	1.53
1	A	19	UFT	O2-C2	-2.33	1.18	1.23
1	B	182	UFT	C2'-C1'	-2.32	1.50	1.53
1	A	215	UFT	O2-C2	-2.32	1.18	1.23
1	B	549	UFT	C2'-C1'	-2.32	1.50	1.53
1	A	182	UFT	C2'-C1'	-2.32	1.50	1.53
1	B	174	UFT	C2'-C1'	-2.32	1.50	1.53
1	B	358	UFT	C2'-C1'	-2.32	1.50	1.53
1	A	555	UFT	O2-C2	-2.31	1.18	1.23
1	B	32	UFT	C2'-C1'	-2.31	1.50	1.53
1	A	472	UFT	C2'-C1'	-2.31	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	523	CFZ	C6-C5	2.31	1.40	1.35
1	B	336	UFT	C2'-C1'	-2.31	1.50	1.53
1	B	305	UFT	O4'-C1'	2.31	1.47	1.42
1	B	19	UFT	O2-C2	-2.30	1.18	1.23
1	A	43	UFT	O2-C2	-2.30	1.18	1.23
1	B	493	UFT	C2'-C1'	-2.30	1.50	1.53
1	B	28	CFZ	C2'-C1'	-2.29	1.50	1.53
1	A	500	UFT	O2-C2	-2.29	1.18	1.23
1	A	305	UFT	O4'-C1'	2.29	1.47	1.42
1	A	350	UFT	O2-C2	-2.29	1.18	1.23
1	B	43	UFT	O2-C2	-2.29	1.18	1.23
1	A	720	UFT	O2-C2	-2.29	1.18	1.23
1	B	48	UFT	O2-C2	-2.29	1.18	1.23
1	A	347	UFT	C2'-C1'	-2.29	1.50	1.53
1	A	182	UFT	O2-C2	-2.28	1.18	1.23
1	B	130	CFZ	C6-C5	2.28	1.40	1.35
1	B	155	UFT	O2-C2	-2.28	1.18	1.23
1	A	687	UFT	O2-C2	-2.28	1.18	1.23
1	B	602	UFT	O2-C2	-2.28	1.18	1.23
1	A	126	UFT	O2-C2	-2.28	1.18	1.23
1	A	689	UFT	O2-C2	-2.28	1.18	1.23
1	A	196	UFT	C2'-C1'	-2.28	1.50	1.53
1	A	447	UFT	O2-C2	-2.28	1.18	1.23
1	B	137	UFT	O2-C2	-2.28	1.18	1.23
1	B	182	UFT	O2-C2	-2.28	1.18	1.23
1	B	214	UFT	O2-C2	-2.28	1.18	1.23
1	A	559	UFT	C2'-C1'	-2.28	1.50	1.53
1	A	472	UFT	O2-C2	-2.27	1.18	1.23
1	B	402	UFT	O2-C2	-2.27	1.18	1.23
1	A	155	UFT	O2-C2	-2.27	1.18	1.23
1	B	322	UFT	O2-C2	-2.27	1.18	1.23
1	B	265	UFT	O2-C2	-2.27	1.18	1.23
1	A	301	UFT	O2-C2	-2.27	1.18	1.23
1	B	245	UFT	O2-C2	-2.27	1.18	1.23
1	A	434	UFT	O2-C2	-2.27	1.18	1.23
1	A	549	UFT	O2-C2	-2.27	1.18	1.23
1	B	676	UFT	O2-C2	-2.27	1.18	1.23
1	B	472	UFT	O2-C2	-2.27	1.18	1.23
1	A	8	UFT	O2-C2	-2.27	1.18	1.23
1	A	214	UFT	O2-C2	-2.27	1.18	1.23
1	A	666	UFT	O2-C2	-2.27	1.18	1.23
1	A	676	UFT	O2-C2	-2.27	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	690	UFT	O2-C2	-2.27	1.18	1.23
1	B	251	UFT	O2-C2	-2.27	1.18	1.23
1	B	635	UFT	O2-C2	-2.27	1.18	1.23
1	A	184	CFZ	C6-C5	2.27	1.40	1.35
1	A	309	UFT	O2-C2	-2.27	1.18	1.23
1	B	14	UFT	O2-C2	-2.27	1.18	1.23
1	A	86	UFT	O2-C2	-2.27	1.18	1.23
1	B	555	UFT	O2-C2	-2.27	1.18	1.23
1	A	581	UFT	O2-C2	-2.27	1.18	1.23
1	B	656	UFT	O2-C2	-2.27	1.18	1.23
1	A	13	UFT	O2-C2	-2.27	1.18	1.23
1	A	282	CFZ	C6-C5	2.27	1.40	1.35
1	B	204	UFT	O2-C2	-2.27	1.18	1.23
1	B	493	UFT	O2-C2	-2.27	1.18	1.23
1	A	97	UFT	O2-C2	-2.26	1.18	1.23
1	A	266	UFT	O2-C2	-2.26	1.18	1.23
1	A	105	UFT	C2'-C1'	-2.26	1.50	1.53
1	B	430	UFT	O2-C2	-2.26	1.18	1.23
1	B	633	UFT	O2-C2	-2.26	1.18	1.23
1	B	108	UFT	O2-C2	-2.26	1.18	1.23
1	B	398	UFT	O2-C2	-2.26	1.18	1.23
1	B	216	UFT	C2'-C1'	-2.26	1.50	1.53
1	B	581	UFT	O2-C2	-2.26	1.18	1.23
1	A	456	UFT	O2-C2	-2.26	1.18	1.23
1	B	590	UFT	O2-C2	-2.26	1.18	1.23
1	A	633	UFT	O2-C2	-2.26	1.18	1.23
1	B	270	UFT	O2-C2	-2.26	1.18	1.23
1	A	153	UFT	O2-C2	-2.26	1.18	1.23
1	A	142	UFT	O2-C2	-2.26	1.18	1.23
1	A	143	UFT	O2-C2	-2.26	1.18	1.23
1	A	251	UFT	O2-C2	-2.26	1.18	1.23
1	B	431	UFT	O2-C2	-2.26	1.18	1.23
1	A	503	UFT	O2-C2	-2.26	1.18	1.23
1	A	353	CFZ	C6-C5	2.26	1.40	1.35
1	B	142	UFT	O2-C2	-2.26	1.18	1.23
1	A	398	UFT	O2-C2	-2.26	1.18	1.23
1	B	519	UFT	O2-C2	-2.26	1.18	1.23
1	B	208	UFT	O2-C2	-2.26	1.18	1.23
1	A	216	UFT	O2-C2	-2.26	1.18	1.23
1	A	629	UFT	O2-C2	-2.26	1.18	1.23
1	B	663	UFT	O2-C2	-2.26	1.18	1.23
1	A	71	UFT	O2-C2	-2.25	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	UFT	O2-C2	-2.25	1.18	1.23
1	B	542	UFT	O2-C2	-2.25	1.18	1.23
1	A	695	UFT	O2-C2	-2.25	1.18	1.23
1	B	106	UFT	O2-C2	-2.25	1.18	1.23
1	A	283	UFT	O2-C2	-2.25	1.18	1.23
1	A	367	UFT	O2-C2	-2.25	1.18	1.23
1	B	524	UFT	O2-C2	-2.25	1.18	1.23
1	B	554	UFT	O2-C2	-2.25	1.18	1.23
1	A	608	UFT	O2-C2	-2.25	1.18	1.23
1	A	494	CFZ	C6-C5	2.25	1.40	1.35
1	A	135	UFT	O2-C2	-2.25	1.18	1.23
1	A	502	UFT	O2-C2	-2.25	1.18	1.23
1	B	719	UFT	O2-C2	-2.25	1.18	1.23
1	A	232	CFZ	C6-C5	2.25	1.40	1.35
1	B	8	UFT	O2-C2	-2.25	1.18	1.23
1	A	365	UFT	O2-C2	-2.25	1.18	1.23
1	A	402	UFT	O2-C2	-2.25	1.18	1.23
1	B	628	UFT	O2-C2	-2.25	1.18	1.23
1	A	254	CFZ	C6-C5	2.25	1.40	1.35
1	B	179	UFT	O2-C2	-2.25	1.18	1.23
1	B	305	UFT	O2-C2	-2.25	1.18	1.23
1	B	336	UFT	O2-C2	-2.25	1.18	1.23
1	A	344	UFT	O2-C2	-2.25	1.18	1.23
1	A	628	UFT	O2-C2	-2.25	1.18	1.23
1	B	687	UFT	O2-C2	-2.25	1.18	1.23
1	A	26	CFZ	C6-C5	2.25	1.40	1.35
1	A	190	UFT	O2-C2	-2.25	1.18	1.23
1	B	621	UFT	O2-C2	-2.25	1.18	1.23
1	A	101	UFT	O2-C2	-2.25	1.18	1.23
1	A	485	UFT	O2-C2	-2.25	1.18	1.23
1	B	582	UFT	O2-C2	-2.25	1.18	1.23
1	B	708	UFT	O2-C2	-2.25	1.18	1.23
1	A	656	UFT	O2-C2	-2.25	1.18	1.23
1	B	673	UFT	O2-C2	-2.25	1.18	1.23
1	B	217	UFT	O2-C2	-2.25	1.18	1.23
1	A	430	UFT	O2-C2	-2.25	1.18	1.23
1	B	62	UFT	O2-C2	-2.25	1.18	1.23
1	A	489	UFT	O2-C2	-2.25	1.18	1.23
1	B	700	CFZ	C6-C5	2.25	1.40	1.35
1	A	432	UFT	O2-C2	-2.25	1.18	1.23
1	A	606	UFT	O2-C2	-2.25	1.18	1.23
1	B	696	UFT	O2-C2	-2.25	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	351	CFZ	C6-C5	2.25	1.40	1.35
1	A	62	UFT	O2-C2	-2.25	1.18	1.23
1	A	163	UFT	O2-C2	-2.25	1.18	1.23
1	A	208	UFT	O2-C2	-2.25	1.18	1.23
1	A	577	UFT	O2-C2	-2.25	1.18	1.23
1	A	245	UFT	O2-C2	-2.25	1.18	1.23
1	A	466	UFT	O2-C2	-2.25	1.18	1.23
1	B	447	UFT	O2-C2	-2.24	1.18	1.23
1	B	460	UFT	O2-C2	-2.24	1.18	1.23
1	B	232	CFZ	C6-C5	2.24	1.40	1.35
1	A	197	UFT	O2-C2	-2.24	1.18	1.23
1	B	500	UFT	O2-C2	-2.24	1.18	1.23
1	A	509	UFT	O2-C2	-2.24	1.18	1.23
1	B	636	UFT	O2-C2	-2.24	1.18	1.23
1	A	114	CFZ	C6-C5	2.24	1.40	1.35
1	A	204	UFT	O2-C2	-2.24	1.18	1.23
1	A	534	UFT	O2-C2	-2.24	1.18	1.23
1	B	59	UFT	O2-C2	-2.24	1.18	1.23
1	B	126	UFT	O2-C2	-2.24	1.18	1.23
1	B	160	UFT	O2-C2	-2.24	1.18	1.23
1	B	367	UFT	O2-C2	-2.24	1.18	1.23
1	B	689	UFT	O2-C2	-2.24	1.18	1.23
1	B	712	UFT	O2-C2	-2.24	1.18	1.23
1	B	212	CFZ	C6-C5	2.24	1.40	1.35
1	B	655	CFZ	C6-C5	2.24	1.40	1.35
1	A	48	UFT	O2-C2	-2.24	1.18	1.23
1	B	50	UFT	O2-C2	-2.24	1.18	1.23
1	B	369	CFZ	C6-C5	2.24	1.40	1.35
1	B	92	UFT	O2-C2	-2.24	1.19	1.23
1	A	137	UFT	O2-C2	-2.24	1.19	1.23
1	B	587	CFZ	C6-C5	2.24	1.40	1.35
1	A	106	UFT	O2-C2	-2.24	1.19	1.23
1	B	313	UFT	O2-C2	-2.24	1.19	1.23
1	A	352	UFT	O2-C2	-2.24	1.19	1.23
1	A	621	UFT	O2-C2	-2.24	1.19	1.23
1	B	662	UFT	O2-C2	-2.24	1.19	1.23
1	A	323	CFZ	C6-C5	2.24	1.40	1.35
1	A	565	CFZ	C6-C5	2.24	1.40	1.35
1	B	404	CFZ	C6-C5	2.24	1.40	1.35
1	B	101	UFT	O2-C2	-2.24	1.19	1.23
1	B	309	UFT	O2-C2	-2.24	1.19	1.23
1	A	115	UFT	O2-C2	-2.24	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79	CFZ	C6-C5	2.24	1.40	1.35
1	A	592	CFZ	C6-C5	2.24	1.40	1.35
1	A	44	UFT	O2-C2	-2.24	1.19	1.23
1	A	169	UFT	O2-C2	-2.24	1.19	1.23
1	A	336	UFT	O2-C2	-2.24	1.19	1.23
1	B	608	UFT	O2-C2	-2.24	1.19	1.23
1	B	669	UFT	O2-C2	-2.24	1.19	1.23
1	B	491	CFZ	C6-C5	2.24	1.40	1.35
1	A	667	CFZ	C6-C5	2.24	1.40	1.35
1	A	59	UFT	O2-C2	-2.24	1.19	1.23
1	B	421	UFT	O2-C2	-2.24	1.19	1.23
1	B	423	UFT	O2-C2	-2.24	1.19	1.23
1	B	666	UFT	O2-C2	-2.24	1.19	1.23
1	B	418	CFZ	C6-C5	2.24	1.40	1.35
1	B	13	UFT	O2-C2	-2.24	1.19	1.23
1	A	593	UFT	O2-C2	-2.24	1.19	1.23
1	A	404	CFZ	C6-C5	2.24	1.40	1.35
1	A	11	UFT	O2-C2	-2.24	1.19	1.23
1	B	55	UFT	O2-C2	-2.24	1.19	1.23
1	B	534	UFT	O2-C2	-2.24	1.19	1.23
1	A	140	CFZ	C6-C5	2.23	1.40	1.35
1	B	190	UFT	O2-C2	-2.23	1.19	1.23
1	B	465	CFZ	C6-C5	2.23	1.40	1.35
1	B	61	UFT	O2-C2	-2.23	1.19	1.23
1	B	80	UFT	O2-C2	-2.23	1.19	1.23
1	B	97	UFT	O2-C2	-2.23	1.19	1.23
1	B	154	UFT	O2-C2	-2.23	1.19	1.23
1	A	646	UFT	O2-C2	-2.23	1.19	1.23
1	B	360	CFZ	C6-C5	2.23	1.40	1.35
1	A	403	UFT	O2-C2	-2.23	1.19	1.23
1	A	421	UFT	O2-C2	-2.23	1.19	1.23
1	B	143	UFT	O2-C2	-2.23	1.19	1.23
1	B	301	UFT	O2-C2	-2.23	1.19	1.23
1	B	347	UFT	O2-C2	-2.23	1.19	1.23
1	A	582	UFT	O2-C2	-2.23	1.19	1.23
1	A	76	CFZ	C6-C5	2.23	1.40	1.35
1	A	474	CFZ	C6-C5	2.23	1.40	1.35
1	B	323	CFZ	C6-C5	2.23	1.40	1.35
1	A	32	UFT	O2-C2	-2.23	1.19	1.23
1	B	71	UFT	O2-C2	-2.23	1.19	1.23
1	B	196	UFT	O2-C2	-2.23	1.19	1.23
1	A	296	UFT	O2-C2	-2.23	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	UFT	O2-C2	-2.23	1.19	1.23
1	B	112	UFT	O2-C2	-2.23	1.19	1.23
1	B	169	UFT	O2-C2	-2.23	1.19	1.23
1	B	577	UFT	O2-C2	-2.23	1.19	1.23
1	B	651	CFZ	C6-C5	2.23	1.40	1.35
1	B	667	CFZ	C6-C5	2.23	1.40	1.35
1	B	202	UFT	O2-C2	-2.23	1.19	1.23
1	A	460	UFT	O2-C2	-2.23	1.19	1.23
1	A	719	UFT	O2-C2	-2.23	1.19	1.23
1	B	399	CFZ	C6-C5	2.23	1.40	1.35
1	A	381	CFZ	C6-C5	2.23	1.40	1.35
1	A	620	CFZ	C6-C5	2.23	1.40	1.35
1	A	481	UFT	O2-C2	-2.23	1.19	1.23
1	B	502	UFT	O2-C2	-2.23	1.19	1.23
1	B	607	UFT	O2-C2	-2.23	1.19	1.23
1	B	116	UFT	O2-C2	-2.23	1.19	1.23
1	B	559	UFT	O2-C2	-2.23	1.19	1.23
1	B	609	UFT	O2-C2	-2.23	1.19	1.23
1	A	673	UFT	O2-C2	-2.23	1.19	1.23
1	B	105	UFT	C2'-C1'	-2.23	1.50	1.53
1	B	618	UFT	O2-C2	-2.23	1.19	1.23
1	B	473	CFZ	C6-C5	2.23	1.40	1.35
1	B	175	UFT	O2-C2	-2.23	1.19	1.23
1	A	112	UFT	O2-C2	-2.23	1.19	1.23
1	B	266	UFT	O2-C2	-2.23	1.19	1.23
1	B	86	UFT	O2-C2	-2.23	1.19	1.23
1	A	92	UFT	O2-C2	-2.23	1.19	1.23
1	A	519	UFT	O2-C2	-2.23	1.19	1.23
1	A	265	UFT	O2-C2	-2.23	1.19	1.23
1	A	493	UFT	O2-C2	-2.23	1.19	1.23
1	B	684	UFT	O2-C2	-2.23	1.19	1.23
1	A	382	CFZ	C6-C5	2.23	1.40	1.35
1	B	192	UFT	O2-C2	-2.23	1.19	1.23
1	B	456	UFT	O2-C2	-2.23	1.19	1.23
1	A	691	CFZ	C6-C5	2.23	1.40	1.35
1	A	437	UFT	O2-C2	-2.23	1.19	1.23
1	A	635	UFT	O2-C2	-2.23	1.19	1.23
1	A	79	CFZ	C6-C5	2.23	1.40	1.35
1	A	458	CFZ	C6-C5	2.23	1.40	1.35
1	A	469	CFZ	C6-C5	2.23	1.40	1.35
1	A	154	UFT	O2-C2	-2.23	1.19	1.23
1	A	587	CFZ	C6-C5	2.22	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	UFT	O2-C2	-2.22	1.19	1.23
1	A	202	UFT	O2-C2	-2.22	1.19	1.23
1	B	361	UFT	O2-C2	-2.22	1.19	1.23
1	B	184	CFZ	C6-C5	2.22	1.40	1.35
1	B	486	CFZ	C6-C5	2.22	1.40	1.35
1	A	662	UFT	O2-C2	-2.22	1.19	1.23
1	B	76	CFZ	C6-C5	2.22	1.40	1.35
1	B	104	CFZ	C6-C5	2.22	1.40	1.35
1	A	558	CFZ	C6-C5	2.22	1.40	1.35
1	A	89	UFT	O2-C2	-2.22	1.19	1.23
1	B	135	UFT	O2-C2	-2.22	1.19	1.23
1	B	229	UFT	O2-C2	-2.22	1.19	1.23
1	A	618	UFT	O2-C2	-2.22	1.19	1.23
1	A	708	UFT	O2-C2	-2.22	1.19	1.23
1	B	96	CFZ	C6-C5	2.22	1.40	1.35
1	A	94	UFT	O2-C2	-2.22	1.19	1.23
1	B	296	UFT	O2-C2	-2.22	1.19	1.23
1	A	524	UFT	O2-C2	-2.22	1.19	1.23
1	A	602	UFT	O2-C2	-2.22	1.19	1.23
1	B	426	CFZ	C6-C5	2.22	1.40	1.35
1	B	583	CFZ	C6-C5	2.22	1.40	1.35
1	B	170	UFT	O2-C2	-2.22	1.19	1.23
1	A	192	UFT	O2-C2	-2.22	1.19	1.23
1	B	344	UFT	O2-C2	-2.22	1.19	1.23
1	A	590	UFT	O2-C2	-2.22	1.19	1.23
1	A	369	CFZ	C6-C5	2.22	1.40	1.35
1	A	451	CFZ	C6-C5	2.22	1.40	1.35
1	B	89	UFT	O2-C2	-2.22	1.19	1.23
1	A	108	UFT	O2-C2	-2.22	1.19	1.23
1	B	434	UFT	O2-C2	-2.22	1.19	1.23
1	A	653	UFT	O2-C2	-2.22	1.19	1.23
1	A	362	CFZ	C6-C5	2.22	1.40	1.35
1	A	604	CFZ	C6-C5	2.22	1.40	1.35
1	A	233	UFT	O2-C2	-2.22	1.19	1.23
1	A	542	UFT	O2-C2	-2.22	1.19	1.23
1	A	571	UFT	O2-C2	-2.22	1.19	1.23
1	B	209	CFZ	C6-C5	2.22	1.40	1.35
1	A	444	CFZ	C6-C5	2.22	1.40	1.35
1	A	700	CFZ	C6-C5	2.22	1.40	1.35
1	B	11	UFT	O2-C2	-2.22	1.19	1.23
1	A	217	UFT	O2-C2	-2.22	1.19	1.23
1	B	690	UFT	O2-C2	-2.22	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	CFZ	C6-C5	2.22	1.40	1.35
1	B	556	CFZ	C6-C5	2.22	1.40	1.35
1	B	603	CFZ	C6-C5	2.22	1.40	1.35
1	B	610	CFZ	C6-C5	2.22	1.40	1.35
1	A	632	CFZ	C6-C5	2.22	1.40	1.35
1	B	72	CFZ	C6-C5	2.22	1.40	1.35
1	A	441	CFZ	C6-C5	2.22	1.40	1.35
1	A	517	CFZ	C6-C5	2.22	1.40	1.35
1	B	637	CFZ	C6-C5	2.22	1.40	1.35
1	A	61	UFT	O2-C2	-2.22	1.19	1.23
1	B	200	UFT	O2-C2	-2.22	1.19	1.23
1	A	366	UFT	O2-C2	-2.22	1.19	1.23
1	B	504	UFT	O2-C2	-2.22	1.19	1.23
1	B	74	UFT	O2-C2	-2.22	1.19	1.23
1	B	403	UFT	O2-C2	-2.22	1.19	1.23
1	B	606	UFT	O2-C2	-2.22	1.19	1.23
1	A	171	CFZ	C6-C5	2.22	1.40	1.35
1	B	620	CFZ	C6-C5	2.22	1.40	1.35
1	B	695	UFT	O2-C2	-2.22	1.19	1.23
1	B	111	CFZ	C6-C5	2.22	1.40	1.35
1	A	511	CFZ	C6-C5	2.22	1.40	1.35
1	A	652	CFZ	C6-C5	2.22	1.40	1.35
1	A	73	CFZ	C6-C5	2.22	1.40	1.35
1	B	353	CFZ	C6-C5	2.22	1.40	1.35
1	A	384	CFZ	C6-C5	2.22	1.40	1.35
1	A	637	CFZ	C6-C5	2.22	1.40	1.35
1	A	355	CFZ	C6-C5	2.22	1.40	1.35
1	B	682	CFZ	C6-C5	2.22	1.40	1.35
1	A	334	UFT	O2-C2	-2.22	1.19	1.23
1	A	696	UFT	O2-C2	-2.22	1.19	1.23
1	A	543	CFZ	C6-C5	2.22	1.40	1.35
1	B	550	CFZ	C6-C5	2.22	1.40	1.35
1	A	175	UFT	O2-C2	-2.22	1.19	1.23
1	A	413	UFT	O2-C2	-2.22	1.19	1.23
1	B	432	UFT	O2-C2	-2.22	1.19	1.23
1	B	198	CFZ	C6-C5	2.22	1.40	1.35
1	B	440	CFZ	C6-C5	2.22	1.40	1.35
1	A	473	CFZ	C6-C5	2.22	1.40	1.35
1	A	50	UFT	O2-C2	-2.22	1.19	1.23
1	A	88	UFT	O2-C2	-2.22	1.19	1.23
1	B	544	UFT	O2-C2	-2.22	1.19	1.23
1	A	554	UFT	O2-C2	-2.22	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	CFZ	C6-C5	2.22	1.40	1.35
1	A	328	CFZ	C6-C5	2.22	1.40	1.35
1	A	440	CFZ	C6-C5	2.22	1.40	1.35
1	A	462	CFZ	C6-C5	2.22	1.40	1.35
1	A	74	UFT	O2-C2	-2.22	1.19	1.23
1	A	431	UFT	O2-C2	-2.22	1.19	1.23
1	A	651	CFZ	C6-C5	2.22	1.40	1.35
1	B	115	UFT	O2-C2	-2.22	1.19	1.23
1	B	174	UFT	O2-C2	-2.22	1.19	1.23
1	A	229	UFT	O2-C2	-2.22	1.19	1.23
1	B	481	UFT	O2-C2	-2.22	1.19	1.23
1	A	513	UFT	O2-C2	-2.22	1.19	1.23
1	B	530	UFT	O2-C2	-2.22	1.19	1.23
1	A	210	CFZ	C6-C5	2.22	1.40	1.35
1	B	574	CFZ	C6-C5	2.22	1.40	1.35
1	B	215	UFT	O2-C2	-2.22	1.19	1.23
1	A	361	UFT	O2-C2	-2.22	1.19	1.23
1	B	593	UFT	O2-C2	-2.22	1.19	1.23
1	A	25	CFZ	C6-C5	2.22	1.40	1.35
1	B	151	CFZ	C6-C5	2.22	1.40	1.35
1	B	406	CFZ	C6-C5	2.22	1.40	1.35
1	B	464	UFT	O2-C2	-2.22	1.19	1.23
1	A	198	CFZ	C6-C5	2.21	1.40	1.35
1	A	436	CFZ	C6-C5	2.21	1.40	1.35
1	A	536	CFZ	C6-C5	2.21	1.40	1.35
1	B	579	CFZ	C6-C5	2.21	1.40	1.35
1	A	603	CFZ	C6-C5	2.21	1.40	1.35
1	B	84	UFT	O2-C2	-2.21	1.19	1.23
1	B	63	CFZ	C6-C5	2.21	1.40	1.35
1	B	691	CFZ	C6-C5	2.21	1.40	1.35
1	A	200	UFT	O2-C2	-2.21	1.19	1.23
1	B	600	CFZ	C6-C5	2.21	1.40	1.35
1	A	607	UFT	O2-C2	-2.21	1.19	1.23
1	A	332	CFZ	C6-C5	2.21	1.40	1.35
1	B	354	CFZ	C6-C5	2.21	1.40	1.35
1	A	600	CFZ	C6-C5	2.21	1.40	1.35
1	B	604	CFZ	C6-C5	2.21	1.40	1.35
1	A	329	UFT	O2-C2	-2.21	1.19	1.23
1	A	712	UFT	O2-C2	-2.21	1.19	1.23
1	A	576	CFZ	C6-C5	2.21	1.40	1.35
1	A	504	UFT	O2-C2	-2.21	1.19	1.23
1	B	90	CFZ	C6-C5	2.21	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	CFZ	C6-C5	2.21	1.40	1.35
1	A	60	UFT	O2-C2	-2.21	1.19	1.23
1	B	69	UFT	O2-C2	-2.21	1.19	1.23
1	A	636	UFT	O2-C2	-2.21	1.19	1.23
1	B	131	CFZ	C6-C5	2.21	1.40	1.35
1	A	579	CFZ	C6-C5	2.21	1.40	1.35
1	A	585	CFZ	C6-C5	2.21	1.40	1.35
1	B	632	CFZ	C6-C5	2.21	1.40	1.35
1	A	347	UFT	O2-C2	-2.21	1.19	1.23
1	B	499	UFT	O2-C2	-2.21	1.19	1.23
1	A	399	CFZ	C6-C5	2.21	1.40	1.35
1	B	411	CFZ	C6-C5	2.21	1.40	1.35
1	B	543	CFZ	C6-C5	2.21	1.40	1.35
1	B	458	CFZ	C6-C5	2.21	1.40	1.35
1	A	130	CFZ	C6-C5	2.21	1.40	1.35
1	B	144	CFZ	C6-C5	2.21	1.40	1.35
1	B	407	CFZ	C6-C5	2.21	1.40	1.35
1	B	233	UFT	O2-C2	-2.21	1.19	1.23
1	B	139	CFZ	C6-C5	2.21	1.40	1.35
1	B	216	UFT	O2-C2	-2.21	1.19	1.23
1	A	663	UFT	O2-C2	-2.21	1.19	1.23
1	B	171	CFZ	C6-C5	2.21	1.40	1.35
1	A	406	CFZ	C6-C5	2.21	1.40	1.35
1	A	196	UFT	O2-C2	-2.21	1.19	1.23
1	B	545	UFT	O2-C2	-2.21	1.19	1.23
1	A	151	CFZ	C6-C5	2.21	1.40	1.35
1	A	655	CFZ	C6-C5	2.21	1.40	1.35
1	A	305	UFT	O2-C2	-2.21	1.19	1.23
1	A	471	UFT	O2-C2	-2.21	1.19	1.23
1	A	72	CFZ	C6-C5	2.21	1.40	1.35
1	A	161	CFZ	C6-C5	2.21	1.40	1.35
1	B	247	CFZ	C6-C5	2.21	1.40	1.35
1	A	438	CFZ	C6-C5	2.21	1.40	1.35
1	A	512	CFZ	C6-C5	2.21	1.40	1.35
1	A	698	CFZ	C6-C5	2.21	1.40	1.35
1	B	437	UFT	O2-C2	-2.21	1.19	1.23
1	B	149	CFZ	C6-C5	2.21	1.40	1.35
1	A	486	CFZ	C6-C5	2.21	1.40	1.35
1	A	506	CFZ	C6-C5	2.21	1.40	1.35
1	A	639	CFZ	C6-C5	2.21	1.40	1.35
1	B	42	UFT	O2-C2	-2.21	1.19	1.23
1	B	141	UFT	O2-C2	-2.21	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	CFZ	C6-C5	2.21	1.40	1.35
1	A	219	CFZ	C6-C5	2.21	1.40	1.35
1	A	455	CFZ	C6-C5	2.21	1.40	1.35
1	B	474	CFZ	C6-C5	2.21	1.40	1.35
1	A	110	CFZ	C6-C5	2.21	1.40	1.35
1	A	144	CFZ	C6-C5	2.21	1.40	1.35
1	A	417	CFZ	C6-C5	2.21	1.40	1.35
1	A	179	UFT	O2-C2	-2.21	1.19	1.23
1	B	15	CFZ	C6-C5	2.21	1.40	1.35
1	B	21	CFZ	C6-C5	2.21	1.40	1.35
1	B	57	CFZ	C6-C5	2.21	1.40	1.35
1	B	218	CFZ	C6-C5	2.21	1.40	1.35
1	B	268	CFZ	C6-C5	2.21	1.40	1.35
1	B	328	CFZ	C6-C5	2.21	1.40	1.35
1	A	160	UFT	O2-C2	-2.21	1.19	1.23
1	A	260	UFT	O2-C2	-2.21	1.19	1.23
1	A	669	UFT	O2-C2	-2.21	1.19	1.23
1	A	293	UFT	O2-C2	-2.21	1.19	1.23
1	A	464	UFT	O2-C2	-2.21	1.19	1.23
1	B	653	UFT	O2-C2	-2.21	1.19	1.23
1	A	703	UFT	O2-C2	-2.21	1.19	1.23
1	A	548	CFZ	C6-C5	2.21	1.40	1.35
1	B	657	CFZ	C6-C5	2.21	1.40	1.35
1	A	270	UFT	O2-C2	-2.21	1.19	1.23
1	B	75	CFZ	C6-C5	2.21	1.40	1.35
1	B	219	CFZ	C6-C5	2.21	1.40	1.35
1	A	370	CFZ	C6-C5	2.21	1.40	1.35
1	B	405	CFZ	C6-C5	2.21	1.40	1.35
1	B	321	CFZ	C6-C5	2.20	1.40	1.35
1	A	664	CFZ	C6-C5	2.20	1.40	1.35
1	B	153	UFT	O2-C2	-2.20	1.19	1.23
1	B	629	UFT	O2-C2	-2.20	1.19	1.23
1	B	164	CFZ	C6-C5	2.20	1.40	1.35
1	B	246	CFZ	C6-C5	2.20	1.40	1.35
1	B	254	CFZ	C6-C5	2.20	1.40	1.35
1	B	511	CFZ	C6-C5	2.20	1.40	1.35
1	A	682	CFZ	C6-C5	2.20	1.40	1.35
1	B	720	UFT	O2-C2	-2.20	1.19	1.23
1	B	26	CFZ	C6-C5	2.20	1.40	1.35
1	B	304	CFZ	C6-C5	2.20	1.40	1.35
1	A	657	CFZ	C6-C5	2.20	1.40	1.35
1	A	246	CFZ	C6-C5	2.20	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	UFT	O2-C2	-2.20	1.19	1.23
1	A	157	CFZ	C6-C5	2.20	1.40	1.35
1	A	164	CFZ	C6-C5	2.20	1.40	1.35
1	B	249	CFZ	C6-C5	2.20	1.40	1.35
1	A	693	CFZ	C6-C5	2.20	1.40	1.35
1	B	438	CFZ	C6-C5	2.20	1.40	1.35
1	B	44	UFT	O2-C2	-2.20	1.19	1.23
1	A	84	UFT	O2-C2	-2.20	1.19	1.23
1	B	466	UFT	O2-C2	-2.20	1.19	1.23
1	A	111	CFZ	C6-C5	2.20	1.40	1.35
1	B	234	CFZ	C6-C5	2.20	1.40	1.35
1	B	381	CFZ	C6-C5	2.20	1.40	1.35
1	A	407	CFZ	C6-C5	2.20	1.40	1.35
1	B	679	CFZ	C6-C5	2.20	1.40	1.35
1	B	698	CFZ	C6-C5	2.20	1.40	1.35
1	A	354	CFZ	C6-C5	2.20	1.40	1.35
1	B	441	CFZ	C6-C5	2.20	1.40	1.35
1	B	293	UFT	O2-C2	-2.20	1.19	1.23
1	B	279	CFZ	C6-C5	2.20	1.40	1.35
1	B	417	CFZ	C6-C5	2.20	1.40	1.35
1	A	625	CFZ	C6-C5	2.20	1.40	1.35
1	B	631	CFZ	C6-C5	2.20	1.40	1.35
1	B	377	UFT	O2-C2	-2.20	1.19	1.23
1	A	423	UFT	O2-C2	-2.20	1.19	1.23
1	B	117	CFZ	C6-C5	2.20	1.40	1.35
1	A	249	CFZ	C6-C5	2.20	1.40	1.35
1	B	334	UFT	O2-C2	-2.20	1.19	1.23
1	A	701	UFT	O2-C2	-2.20	1.19	1.23
1	B	512	CFZ	C6-C5	2.20	1.40	1.35
1	A	631	CFZ	C6-C5	2.20	1.40	1.35
1	B	652	CFZ	C6-C5	2.20	1.40	1.35
1	B	664	CFZ	C6-C5	2.20	1.40	1.35
1	B	471	UFT	O2-C2	-2.20	1.19	1.23
1	A	316	CFZ	C6-C5	2.20	1.40	1.35
1	A	540	CFZ	C6-C5	2.20	1.40	1.35
1	B	282	CFZ	C6-C5	2.20	1.40	1.35
1	A	360	CFZ	C6-C5	2.20	1.40	1.35
1	B	378	CFZ	C6-C5	2.20	1.40	1.35
1	A	583	CFZ	C6-C5	2.20	1.40	1.35
1	B	32	UFT	O2-C2	-2.20	1.19	1.23
1	B	60	UFT	O2-C2	-2.20	1.19	1.23
1	A	69	UFT	O2-C2	-2.20	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	509	UFT	O2-C2	-2.20	1.19	1.23
1	A	349	CFZ	C6-C5	2.20	1.40	1.35
1	B	535	UFT	O2-C2	-2.20	1.19	1.23
1	A	378	CFZ	C6-C5	2.20	1.40	1.35
1	B	446	CFZ	C6-C5	2.20	1.40	1.35
1	B	549	UFT	O2-C2	-2.20	1.19	1.23
1	A	103	CFZ	C6-C5	2.20	1.40	1.35
1	B	528	CFZ	C6-C5	2.20	1.40	1.35
1	B	704	CFZ	C6-C5	2.20	1.40	1.35
1	A	313	UFT	O2-C2	-2.20	1.19	1.23
1	B	359	UFT	O2-C2	-2.20	1.19	1.23
1	B	241	CFZ	C6-C5	2.20	1.40	1.35
1	A	373	CFZ	C6-C5	2.20	1.40	1.35
1	A	498	CFZ	C6-C5	2.20	1.40	1.35
1	A	564	CFZ	C6-C5	2.20	1.40	1.35
1	B	98	UFT	O2-C2	-2.20	1.19	1.23
1	A	170	UFT	O2-C2	-2.20	1.19	1.23
1	A	545	UFT	O2-C2	-2.20	1.19	1.23
1	A	559	UFT	O2-C2	-2.20	1.19	1.23
1	B	67	CFZ	C6-C5	2.20	1.40	1.35
1	B	298	CFZ	C6-C5	2.20	1.40	1.35
1	B	518	CFZ	C6-C5	2.20	1.40	1.35
1	A	28	CFZ	C6-C5	2.19	1.40	1.35
1	A	418	CFZ	C6-C5	2.19	1.40	1.35
1	B	540	CFZ	C6-C5	2.19	1.40	1.35
1	B	88	UFT	O2-C2	-2.19	1.19	1.23
1	B	352	UFT	O2-C2	-2.19	1.19	1.23
1	B	701	UFT	O2-C2	-2.19	1.19	1.23
1	A	63	CFZ	C6-C5	2.19	1.40	1.35
1	A	90	CFZ	C6-C5	2.19	1.40	1.35
1	B	120	CFZ	C6-C5	2.19	1.40	1.35
1	B	643	CFZ	C6-C5	2.19	1.40	1.35
1	A	174	UFT	O2-C2	-2.19	1.19	1.23
1	B	10	CFZ	C6-C5	2.19	1.40	1.35
1	B	363	CFZ	C6-C5	2.19	1.40	1.35
1	B	551	CFZ	C6-C5	2.19	1.40	1.35
1	A	679	CFZ	C6-C5	2.19	1.40	1.35
1	B	459	CFZ	C6-C5	2.19	1.40	1.35
1	B	210	CFZ	C6-C5	2.19	1.40	1.35
1	B	362	CFZ	C6-C5	2.19	1.40	1.35
1	A	439	CFZ	C6-C5	2.19	1.40	1.35
1	A	34	CFZ	C6-C5	2.19	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	315	CFZ	C6-C5	2.19	1.40	1.35
1	A	610	CFZ	C6-C5	2.19	1.40	1.35
1	A	377	UFT	O2-C2	-2.19	1.19	1.23
1	A	609	UFT	O2-C2	-2.19	1.19	1.23
1	A	129	CFZ	C6-C5	2.19	1.40	1.35
1	A	209	CFZ	C6-C5	2.19	1.40	1.35
1	A	363	CFZ	C6-C5	2.19	1.40	1.35
1	A	268	CFZ	C6-C5	2.19	1.40	1.35
1	A	10	CFZ	C6-C5	2.19	1.40	1.35
1	A	96	CFZ	C6-C5	2.19	1.40	1.35
1	A	242	CFZ	C6-C5	2.19	1.40	1.35
1	A	285	CFZ	C6-C5	2.19	1.40	1.35
1	B	564	CFZ	C6-C5	2.19	1.40	1.35
1	B	260	UFT	O2-C2	-2.19	1.19	1.23
1	A	325	CFZ	C6-C5	2.19	1.40	1.35
1	A	424	CFZ	C6-C5	2.19	1.40	1.35
1	B	33	UFT	O2-C2	-2.19	1.19	1.23
1	A	98	UFT	O2-C2	-2.19	1.19	1.23
1	A	57	CFZ	C6-C5	2.19	1.40	1.35
1	A	212	CFZ	C6-C5	2.19	1.40	1.35
1	A	614	CFZ	C6-C5	2.19	1.40	1.35
1	B	485	UFT	O2-C2	-2.19	1.19	1.23
1	A	535	UFT	O2-C2	-2.19	1.19	1.23
1	B	659	UFT	O2-C2	-2.19	1.19	1.23
1	A	315	CFZ	C6-C5	2.19	1.40	1.35
1	A	491	CFZ	C6-C5	2.19	1.40	1.35
1	B	517	CFZ	C6-C5	2.19	1.40	1.35
1	A	42	UFT	O2-C2	-2.19	1.19	1.23
1	B	365	UFT	O2-C2	-2.19	1.19	1.23
1	A	304	CFZ	C6-C5	2.19	1.40	1.35
1	B	332	CFZ	C6-C5	2.19	1.40	1.35
1	B	384	CFZ	C6-C5	2.19	1.40	1.35
1	B	536	CFZ	C6-C5	2.19	1.40	1.35
1	B	358	UFT	O2-C2	-2.19	1.19	1.23
1	B	383	CFZ	C6-C5	2.19	1.40	1.35
1	A	389	UFT	O2-C2	-2.19	1.19	1.23
1	B	325	CFZ	C6-C5	2.19	1.40	1.35
1	A	477	CFZ	C6-C5	2.19	1.40	1.35
1	A	156	CFZ	C6-C5	2.19	1.40	1.35
1	B	316	CFZ	C6-C5	2.19	1.40	1.35
1	A	528	CFZ	C6-C5	2.19	1.40	1.35
1	A	247	CFZ	C6-C5	2.19	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	CFZ	C6-C5	2.19	1.40	1.35
1	B	614	CFZ	C6-C5	2.19	1.40	1.35
1	B	197	UFT	O2-C2	-2.19	1.19	1.23
1	B	73	CFZ	C6-C5	2.19	1.40	1.35
1	A	117	CFZ	C6-C5	2.19	1.40	1.35
1	B	140	CFZ	C6-C5	2.19	1.40	1.35
1	A	201	CFZ	C6-C5	2.19	1.40	1.35
1	A	459	CFZ	C6-C5	2.19	1.40	1.35
1	B	571	UFT	O2-C2	-2.19	1.19	1.23
1	B	387	CFZ	C6-C5	2.19	1.40	1.35
1	B	565	CFZ	C6-C5	2.19	1.40	1.35
1	B	329	UFT	O2-C2	-2.18	1.19	1.23
1	B	389	UFT	O2-C2	-2.18	1.19	1.23
1	B	639	CFZ	C6-C5	2.18	1.40	1.35
1	A	49	CFZ	C6-C5	2.18	1.40	1.35
1	A	139	CFZ	C6-C5	2.18	1.40	1.35
1	B	201	CFZ	C6-C5	2.18	1.40	1.35
1	A	321	CFZ	C6-C5	2.18	1.40	1.35
1	B	548	CFZ	C6-C5	2.18	1.40	1.35
1	A	141	UFT	O2-C2	-2.18	1.19	1.23
1	B	646	UFT	O2-C2	-2.18	1.19	1.23
1	A	465	CFZ	C6-C5	2.18	1.40	1.35
1	A	426	CFZ	C6-C5	2.18	1.40	1.35
1	A	21	CFZ	C6-C5	2.18	1.40	1.35
1	A	104	CFZ	C6-C5	2.18	1.40	1.35
1	B	124	CFZ	C6-C5	2.18	1.40	1.35
1	B	206	CFZ	C6-C5	2.18	1.40	1.35
1	B	105	UFT	O2-C2	-2.18	1.19	1.23
1	B	489	UFT	O2-C2	-2.18	1.19	1.23
1	B	46	CFZ	C6-C5	2.18	1.40	1.35
1	A	298	CFZ	C6-C5	2.18	1.40	1.35
1	A	308	CFZ	C6-C5	2.18	1.40	1.35
1	A	116	UFT	O2-C2	-2.18	1.19	1.23
1	A	544	UFT	O2-C2	-2.18	1.19	1.23
1	A	120	CFZ	C6-C5	2.18	1.40	1.35
1	B	165	CFZ	C6-C5	2.18	1.40	1.35
1	B	469	CFZ	C6-C5	2.18	1.40	1.35
1	B	625	CFZ	C6-C5	2.18	1.40	1.35
1	A	704	CFZ	C6-C5	2.18	1.40	1.35
1	B	506	CFZ	C6-C5	2.18	1.40	1.35
1	A	568	CFZ	C6-C5	2.18	1.40	1.35
1	B	425	CFZ	C6-C5	2.18	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	647	CFZ	C6-C5	2.18	1.40	1.35
1	B	477	CFZ	C6-C5	2.18	1.40	1.35
1	B	114	CFZ	C6-C5	2.18	1.40	1.35
1	B	156	CFZ	C6-C5	2.18	1.40	1.35
1	A	234	CFZ	C6-C5	2.18	1.40	1.35
1	A	206	CFZ	C6-C5	2.18	1.40	1.35
1	B	355	CFZ	C6-C5	2.18	1.40	1.35
1	A	214	UFT	C2'-C1'	-2.18	1.50	1.53
1	A	372	CFZ	C6-C5	2.18	1.40	1.35
1	B	103	CFZ	C6-C5	2.18	1.40	1.35
1	B	173	CFZ	C6-C5	2.18	1.40	1.35
1	B	373	CFZ	C6-C5	2.18	1.40	1.35
1	B	302	UFT	O2-C2	-2.18	1.19	1.23
1	B	703	UFT	O2-C2	-2.18	1.19	1.23
1	A	358	UFT	C2'-C1'	-2.18	1.50	1.53
1	B	585	CFZ	C6-C5	2.18	1.40	1.35
1	A	46	CFZ	C6-C5	2.18	1.40	1.35
1	A	241	CFZ	C6-C5	2.18	1.40	1.35
1	B	370	CFZ	C6-C5	2.18	1.40	1.35
1	B	366	UFT	O2-C2	-2.18	1.19	1.23
1	A	67	CFZ	C6-C5	2.17	1.40	1.35
1	A	149	CFZ	C6-C5	2.17	1.40	1.35
1	B	351	CFZ	C6-C5	2.17	1.40	1.35
1	A	173	CFZ	C6-C5	2.17	1.40	1.35
1	B	576	CFZ	C6-C5	2.17	1.40	1.35
1	A	131	CFZ	C6-C5	2.17	1.40	1.35
1	B	439	CFZ	C6-C5	2.17	1.40	1.35
1	B	693	CFZ	C6-C5	2.17	1.40	1.35
1	A	519	UFT	C2'-C1'	-2.17	1.50	1.53
1	A	15	CFZ	C6-C5	2.17	1.40	1.35
1	B	188	CFZ	C6-C5	2.17	1.40	1.35
1	A	551	CFZ	C6-C5	2.17	1.40	1.35
1	A	383	CFZ	C6-C5	2.17	1.40	1.35
1	A	322	UFT	O2-C2	-2.17	1.19	1.23
1	A	75	CFZ	C6-C5	2.17	1.40	1.35
1	B	285	CFZ	C6-C5	2.17	1.40	1.35
1	B	424	CFZ	C6-C5	2.17	1.40	1.35
1	A	302	UFT	O2-C2	-2.17	1.19	1.23
1	B	308	CFZ	C6-C5	2.17	1.40	1.35
1	A	279	CFZ	C6-C5	2.17	1.40	1.35
1	B	338	CFZ	C6-C5	2.17	1.40	1.35
1	A	446	CFZ	C6-C5	2.17	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	CFZ	C6-C5	2.17	1.40	1.35
1	A	684	UFT	O2-C2	-2.17	1.19	1.23
1	A	165	CFZ	C6-C5	2.17	1.40	1.35
1	B	34	CFZ	C6-C5	2.17	1.40	1.35
1	A	518	CFZ	C6-C5	2.16	1.40	1.35
1	A	659	UFT	O2-C2	-2.16	1.19	1.23
1	A	550	CFZ	C6-C5	2.16	1.40	1.35
1	A	643	CFZ	C6-C5	2.16	1.40	1.35
1	A	33	UFT	O2-C2	-2.16	1.19	1.23
1	A	425	CFZ	C6-C5	2.16	1.40	1.35
1	A	188	CFZ	C6-C5	2.16	1.40	1.35
1	B	110	CFZ	C6-C5	2.16	1.40	1.35
1	A	218	CFZ	C6-C5	2.16	1.40	1.35
1	A	411	CFZ	C6-C5	2.16	1.40	1.35
1	B	568	CFZ	C6-C5	2.16	1.40	1.35
1	A	556	CFZ	C6-C5	2.16	1.40	1.35
1	B	498	CFZ	C6-C5	2.16	1.40	1.35
1	B	157	CFZ	C6-C5	2.16	1.40	1.35
1	A	574	CFZ	C6-C5	2.16	1.40	1.35
1	B	242	CFZ	C6-C5	2.16	1.40	1.35
1	A	530	UFT	O2-C2	-2.15	1.19	1.23
1	A	80	UFT	O2-C2	-2.15	1.19	1.23
1	A	359	UFT	O2-C2	-2.15	1.19	1.23
1	A	124	CFZ	C6-C5	2.15	1.40	1.35
1	B	592	CFZ	C6-C5	2.15	1.40	1.35
1	B	372	CFZ	C6-C5	2.15	1.40	1.35
1	B	513	UFT	O2-C2	-2.15	1.19	1.23
1	B	558	CFZ	C6-C5	2.14	1.40	1.35
1	B	25	CFZ	C6-C5	2.14	1.40	1.35
1	B	39	CFZ	C6-C5	2.14	1.40	1.35
1	B	647	CFZ	C6-C5	2.14	1.40	1.35
1	A	492	CFZ	C6-C5	2.14	1.40	1.35
1	A	105	UFT	O2-C2	-2.14	1.19	1.23
1	B	49	CFZ	C6-C5	2.14	1.40	1.35
1	A	358	UFT	O2-C2	-2.13	1.19	1.23
1	A	523	CFZ	C6-C5	2.13	1.40	1.35
1	A	39	CFZ	C6-C5	2.13	1.40	1.35
1	B	335	CFZ	C6-C5	2.12	1.39	1.35
1	A	335	CFZ	C6-C5	2.12	1.39	1.35
1	A	359	UFT	C2'-C1'	-2.10	1.50	1.53
1	B	492	CFZ	C6-C5	2.07	1.39	1.35
1	B	89	UFT	C4-N3	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	UFT	C4-N3	2.05	1.42	1.38
1	B	628	UFT	C4-N3	2.05	1.42	1.38
1	A	555	UFT	C4-N3	2.05	1.42	1.38
1	A	98	UFT	C4-N3	2.05	1.42	1.38
1	B	423	UFT	C4-N3	2.05	1.42	1.38
1	B	270	UFT	C4-N3	2.04	1.42	1.38
1	B	336	UFT	C4-N3	2.04	1.42	1.38
1	A	266	UFT	C4-N3	2.04	1.42	1.38
1	B	112	UFT	C4-N3	2.04	1.42	1.38
1	A	69	UFT	C4-N3	2.04	1.42	1.38
1	A	432	UFT	C4-N3	2.04	1.42	1.38
1	B	86	UFT	C4-N3	2.04	1.42	1.38
1	A	534	UFT	C4-N3	2.04	1.42	1.38
1	B	266	UFT	C4-N3	2.04	1.42	1.38
1	A	270	UFT	C4-N3	2.04	1.42	1.38
1	B	142	UFT	C4-N3	2.04	1.42	1.38
1	A	137	UFT	C4-N3	2.04	1.42	1.38
1	A	431	UFT	C4-N3	2.04	1.42	1.38
1	B	296	UFT	C4-N3	2.04	1.42	1.38
1	B	504	UFT	C4-N3	2.03	1.42	1.38
1	B	504	UFT	O5'-C5'	-2.03	1.39	1.44
1	A	112	UFT	C4-N3	2.03	1.42	1.38
1	A	32	UFT	C4-N3	2.03	1.42	1.38
1	B	618	UFT	C4-N3	2.03	1.42	1.38
1	B	202	UFT	C4-N3	2.03	1.42	1.38
1	B	305	UFT	C4-N3	2.03	1.42	1.38
1	A	14	UFT	O5'-C5'	-2.03	1.39	1.44
1	B	712	UFT	C4-N3	2.03	1.42	1.38
1	A	549	UFT	C4-N3	2.03	1.42	1.38
1	B	92	UFT	C4-N3	2.03	1.42	1.38
1	B	154	UFT	C4-N3	2.03	1.42	1.38
1	A	32	UFT	O5'-C5'	-2.03	1.39	1.44
1	A	74	UFT	C4-N3	2.03	1.42	1.38
1	A	689	UFT	C4-N3	2.03	1.42	1.38
1	B	695	UFT	C4-N3	2.03	1.42	1.38
1	B	215	UFT	C4-N3	2.03	1.42	1.38
1	B	402	UFT	C4-N3	2.03	1.42	1.38
1	A	606	UFT	C4-N3	2.03	1.42	1.38
1	B	233	UFT	C4-N3	2.02	1.42	1.38
1	A	402	UFT	C4-N3	2.02	1.42	1.38
1	A	554	UFT	C4-N3	2.02	1.42	1.38
1	B	554	UFT	C4-N3	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	UFT	C4-N3	2.02	1.42	1.38
1	B	170	UFT	C4-N3	2.02	1.42	1.38
1	A	633	UFT	C4-N3	2.02	1.42	1.38
1	B	719	UFT	C4-N3	2.02	1.42	1.38
1	B	606	UFT	C4-N3	2.02	1.42	1.38
1	A	11	UFT	C4-N3	2.02	1.42	1.38
1	A	101	UFT	C4-N3	2.02	1.42	1.38
1	B	301	UFT	C4-N3	2.02	1.42	1.38
1	A	503	UFT	C4-N3	2.02	1.42	1.38
1	A	466	UFT	C4-N3	2.02	1.42	1.38
1	B	359	UFT	C4-N3	2.02	1.42	1.38
1	A	577	UFT	C4-N3	2.02	1.42	1.38
1	B	192	UFT	C4-N3	2.02	1.42	1.38
1	A	59	UFT	C4-N3	2.02	1.42	1.38
1	B	434	UFT	C4-N3	2.02	1.42	1.38
1	A	628	UFT	C4-N3	2.02	1.42	1.38
1	B	403	UFT	C4-N3	2.02	1.42	1.38
1	A	398	UFT	C4-N3	2.02	1.42	1.38
1	B	509	UFT	C4-N3	2.02	1.42	1.38
1	A	559	UFT	C4-N3	2.02	1.42	1.38
1	B	160	UFT	C4-N3	2.02	1.42	1.38
1	A	344	UFT	C4-N3	2.02	1.42	1.38
1	A	609	UFT	C4-N3	2.02	1.42	1.38
1	B	663	UFT	C4-N3	2.02	1.42	1.38
1	A	485	UFT	C4-N3	2.01	1.42	1.38
1	B	502	UFT	C4-N3	2.01	1.42	1.38
1	B	542	UFT	C4-N3	2.01	1.42	1.38
1	A	673	UFT	C4-N3	2.01	1.42	1.38
1	A	84	UFT	C4-N3	2.01	1.42	1.38
1	B	577	UFT	C4-N3	2.01	1.42	1.38
1	B	98	UFT	C4-N3	2.01	1.42	1.38
1	B	200	UFT	C4-N3	2.01	1.42	1.38
1	A	430	UFT	C4-N3	2.01	1.42	1.38
1	B	690	UFT	C4-N3	2.01	1.42	1.38
1	A	192	UFT	C4-N3	2.01	1.42	1.38
1	B	94	UFT	C4-N3	2.01	1.42	1.38
1	A	251	UFT	C4-N3	2.01	1.42	1.38
1	A	403	UFT	C4-N3	2.01	1.42	1.38
1	A	190	UFT	C4-N3	2.01	1.42	1.38
1	B	500	UFT	C4-N3	2.01	1.42	1.38
1	A	571	UFT	C4-N3	2.01	1.42	1.38
1	B	636	UFT	C4-N3	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	421	UFT	C4-N3	2.01	1.42	1.38
1	A	582	UFT	C4-N3	2.01	1.42	1.38
1	B	608	UFT	C4-N3	2.01	1.42	1.38
1	A	719	UFT	C4-N3	2.01	1.42	1.38
1	B	466	UFT	C4-N3	2.01	1.42	1.38
1	B	656	UFT	C4-N3	2.01	1.42	1.38
1	A	86	UFT	C4-N3	2.01	1.42	1.38
1	B	398	UFT	C4-N3	2.01	1.42	1.38
1	B	609	UFT	C4-N3	2.01	1.42	1.38
1	B	666	UFT	C4-N3	2.01	1.42	1.38
1	B	48	UFT	C4-N3	2.01	1.42	1.38
1	A	115	UFT	C4-N3	2.01	1.42	1.38
1	A	169	UFT	C4-N3	2.01	1.42	1.38
1	A	19	UFT	C4-N3	2.01	1.42	1.38
1	A	88	UFT	C4-N3	2.00	1.42	1.38
1	A	635	UFT	C4-N3	2.00	1.42	1.38
1	B	197	UFT	C4-N3	2.00	1.42	1.38
1	B	544	UFT	C4-N3	2.00	1.42	1.38
1	A	8	UFT	C4-N3	2.00	1.42	1.38
1	A	71	UFT	C4-N3	2.00	1.42	1.38
1	B	175	UFT	C4-N3	2.00	1.42	1.38
1	B	251	UFT	C4-N3	2.00	1.42	1.38
1	A	366	UFT	C4-N3	2.00	1.42	1.38
1	B	431	UFT	C4-N3	2.00	1.42	1.38
1	B	534	UFT	C4-N3	2.00	1.42	1.38
1	B	329	UFT	C4-N3	2.00	1.42	1.38
1	A	509	UFT	C4-N3	2.00	1.42	1.38
1	B	633	UFT	C4-N3	2.00	1.42	1.38
1	A	347	UFT	C4-N3	2.00	1.42	1.38
1	B	621	UFT	C4-N3	2.00	1.42	1.38
1	A	504	UFT	O5'-C5'	-2.00	1.39	1.44
1	A	202	UFT	C4-N3	2.00	1.42	1.38
1	A	265	UFT	C4-N3	2.00	1.42	1.38
1	A	602	UFT	C4-N3	2.00	1.42	1.38
1	A	296	UFT	C4-N3	2.00	1.42	1.38
1	A	62	UFT	C4-N3	2.00	1.42	1.38
1	A	500	UFT	C4-N3	2.00	1.42	1.38
1	B	88	UFT	C4-N3	2.00	1.42	1.38
1	B	217	UFT	C4-N3	2.00	1.42	1.38
1	B	492	CFZ	O5'-C5'	-2.00	1.39	1.44

All (3511) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	CFZ	C2'-C1'-N1	-6.31	104.55	114.20
1	A	14	UFT	C4-N3-C2	-5.19	119.73	126.58
1	B	361	UFT	C4-N3-C2	-5.14	119.80	126.58
1	A	350	UFT	C4-N3-C2	-5.12	119.83	126.58
1	A	19	UFT	C4-N3-C2	-5.09	119.86	126.58
1	B	19	UFT	C4-N3-C2	-5.09	119.87	126.58
1	A	347	UFT	C4-N3-C2	-5.09	119.87	126.58
1	B	359	UFT	C4-N3-C2	-5.09	119.87	126.58
1	A	636	UFT	C4-N3-C2	-5.08	119.87	126.58
1	A	142	UFT	C4-N3-C2	-5.08	119.87	126.58
1	B	62	UFT	C4-N3-C2	-5.08	119.88	126.58
1	B	431	UFT	C4-N3-C2	-5.08	119.88	126.58
1	B	434	UFT	C4-N3-C2	-5.08	119.88	126.58
1	A	74	UFT	C4-N3-C2	-5.08	119.88	126.58
1	A	398	UFT	C4-N3-C2	-5.08	119.88	126.58
1	A	403	UFT	C4-N3-C2	-5.08	119.88	126.58
1	B	403	UFT	C4-N3-C2	-5.08	119.88	126.58
1	B	593	UFT	C4-N3-C2	-5.07	119.89	126.58
1	A	301	UFT	C4-N3-C2	-5.07	119.89	126.58
1	B	608	UFT	C4-N3-C2	-5.07	119.89	126.58
1	B	86	UFT	C4-N3-C2	-5.07	119.89	126.58
1	A	170	UFT	C4-N3-C2	-5.07	119.89	126.58
1	B	301	UFT	C4-N3-C2	-5.07	119.89	126.58
1	B	662	UFT	C4-N3-C2	-5.07	119.89	126.58
1	B	160	UFT	C4-N3-C2	-5.07	119.89	126.58
1	A	336	UFT	C4-N3-C2	-5.07	119.89	126.58
1	B	74	UFT	C4-N3-C2	-5.06	119.90	126.58
1	A	61	UFT	C4-N3-C2	-5.06	119.91	126.58
1	B	202	UFT	C4-N3-C2	-5.06	119.91	126.58
1	B	44	UFT	C4-N3-C2	-5.06	119.91	126.58
1	A	283	UFT	C4-N3-C2	-5.06	119.91	126.58
1	B	88	UFT	C4-N3-C2	-5.06	119.91	126.58
1	B	170	UFT	C4-N3-C2	-5.06	119.91	126.58
1	B	336	UFT	C4-N3-C2	-5.06	119.91	126.58
1	B	215	UFT	C4-N3-C2	-5.06	119.91	126.58
1	B	430	UFT	C4-N3-C2	-5.06	119.91	126.58
1	B	666	UFT	C4-N3-C2	-5.06	119.91	126.58
1	A	62	UFT	C4-N3-C2	-5.05	119.91	126.58
1	A	197	UFT	C4-N3-C2	-5.05	119.92	126.58
1	B	313	UFT	C4-N3-C2	-5.05	119.92	126.58
1	A	663	UFT	C4-N3-C2	-5.05	119.92	126.58
1	B	504	UFT	C4-N3-C2	-5.05	119.92	126.58
1	B	296	UFT	C4-N3-C2	-5.05	119.92	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	UFT	C4-N3-C2	-5.05	119.92	126.58
1	A	296	UFT	C4-N3-C2	-5.05	119.92	126.58
1	A	554	UFT	C4-N3-C2	-5.05	119.92	126.58
1	B	116	UFT	C4-N3-C2	-5.05	119.92	126.58
1	B	126	UFT	C4-N3-C2	-5.05	119.92	126.58
1	A	200	UFT	C4-N3-C2	-5.05	119.92	126.58
1	A	621	UFT	C4-N3-C2	-5.05	119.92	126.58
1	B	190	UFT	C4-N3-C2	-5.05	119.92	126.58
1	B	197	UFT	C4-N3-C2	-5.05	119.92	126.58
1	A	690	UFT	C4-N3-C2	-5.05	119.92	126.58
1	A	190	UFT	C4-N3-C2	-5.04	119.93	126.58
1	B	653	UFT	C4-N3-C2	-5.04	119.93	126.58
1	B	61	UFT	C4-N3-C2	-5.04	119.93	126.58
1	B	143	UFT	C4-N3-C2	-5.04	119.93	126.58
1	B	606	UFT	C4-N3-C2	-5.04	119.93	126.58
1	A	154	UFT	C4-N3-C2	-5.04	119.93	126.58
1	B	11	UFT	C4-N3-C2	-5.04	119.93	126.58
1	A	160	UFT	C4-N3-C2	-5.04	119.93	126.58
1	A	582	UFT	C4-N3-C2	-5.04	119.93	126.58
1	B	89	UFT	C4-N3-C2	-5.04	119.93	126.58
1	B	542	UFT	C4-N3-C2	-5.04	119.93	126.58
1	A	270	UFT	C4-N3-C2	-5.04	119.93	126.58
1	B	582	UFT	C4-N3-C2	-5.04	119.93	126.58
1	B	101	UFT	C4-N3-C2	-5.04	119.93	126.58
1	A	430	UFT	C4-N3-C2	-5.04	119.93	126.58
1	B	696	UFT	C4-N3-C2	-5.04	119.94	126.58
1	B	98	UFT	C4-N3-C2	-5.04	119.94	126.58
1	A	89	UFT	C4-N3-C2	-5.04	119.94	126.58
1	B	554	UFT	C4-N3-C2	-5.04	119.94	126.58
1	B	633	UFT	C4-N3-C2	-5.04	119.94	126.58
1	A	32	UFT	C4-N3-C2	-5.04	119.94	126.58
1	A	666	UFT	C4-N3-C2	-5.04	119.94	126.58
1	A	720	UFT	C4-N3-C2	-5.04	119.94	126.58
1	A	86	UFT	C4-N3-C2	-5.03	119.94	126.58
1	B	283	UFT	C4-N3-C2	-5.03	119.94	126.58
1	A	577	UFT	C4-N3-C2	-5.03	119.94	126.58
1	B	609	UFT	C4-N3-C2	-5.03	119.94	126.58
1	A	555	UFT	C4-N3-C2	-5.03	119.94	126.58
1	A	609	UFT	C4-N3-C2	-5.03	119.94	126.58
1	A	143	UFT	C4-N3-C2	-5.03	119.94	126.58
1	B	519	UFT	C4-N3-C2	-5.03	119.94	126.58
1	B	142	UFT	C4-N3-C2	-5.03	119.94	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	UFT	C4-N3-C2	-5.03	119.94	126.58
1	A	202	UFT	C4-N3-C2	-5.03	119.95	126.58
1	A	431	UFT	C4-N3-C2	-5.03	119.95	126.58
1	B	154	UFT	C4-N3-C2	-5.03	119.95	126.58
1	B	155	UFT	C4-N3-C2	-5.03	119.95	126.58
1	A	69	UFT	C4-N3-C2	-5.03	119.95	126.58
1	A	115	UFT	C4-N3-C2	-5.03	119.95	126.58
1	A	116	UFT	C4-N3-C2	-5.03	119.95	126.58
1	B	500	UFT	C4-N3-C2	-5.03	119.95	126.58
1	B	13	UFT	C4-N3-C2	-5.03	119.95	126.58
1	B	14	UFT	C4-N3-C2	-5.03	119.95	126.58
1	B	663	UFT	C4-N3-C2	-5.03	119.95	126.58
1	B	200	UFT	C4-N3-C2	-5.03	119.95	126.58
1	B	466	UFT	C4-N3-C2	-5.03	119.95	126.58
1	B	690	UFT	C4-N3-C2	-5.03	119.95	126.58
1	A	662	UFT	C4-N3-C2	-5.02	119.95	126.58
1	A	493	UFT	C4-N3-C2	-5.02	119.95	126.58
1	A	608	UFT	C4-N3-C2	-5.02	119.95	126.58
1	A	633	UFT	C4-N3-C2	-5.02	119.95	126.58
1	B	94	UFT	C4-N3-C2	-5.02	119.95	126.58
1	B	322	UFT	C4-N3-C2	-5.02	119.95	126.58
1	A	101	UFT	C4-N3-C2	-5.02	119.96	126.58
1	A	265	UFT	C4-N3-C2	-5.02	119.96	126.58
1	A	352	UFT	C4-N3-C2	-5.02	119.96	126.58
1	A	606	UFT	C4-N3-C2	-5.02	119.96	126.58
1	B	182	UFT	C4-N3-C2	-5.02	119.96	126.58
1	B	217	UFT	C4-N3-C2	-5.02	119.96	126.58
1	B	398	UFT	C4-N3-C2	-5.02	119.96	126.58
1	B	636	UFT	C4-N3-C2	-5.02	119.96	126.58
1	A	217	UFT	C4-N3-C2	-5.02	119.96	126.58
1	A	500	UFT	C4-N3-C2	-5.02	119.96	126.58
1	A	696	UFT	C4-N3-C2	-5.02	119.96	126.58
1	A	13	UFT	C4-N3-C2	-5.02	119.96	126.58
1	A	88	UFT	C4-N3-C2	-5.02	119.96	126.58
1	B	265	UFT	C4-N3-C2	-5.02	119.96	126.58
1	A	155	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	437	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	489	UFT	C4-N3-C2	-5.01	119.97	126.58
1	B	270	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	126	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	245	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	504	UFT	C4-N3-C2	-5.01	119.97	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	466	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	519	UFT	C4-N3-C2	-5.01	119.97	126.58
1	B	689	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	542	UFT	C4-N3-C2	-5.01	119.97	126.58
1	B	618	UFT	C4-N3-C2	-5.01	119.97	126.58
1	B	635	UFT	C4-N3-C2	-5.01	119.97	126.58
1	B	112	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	646	UFT	C4-N3-C2	-5.01	119.97	126.58
1	B	530	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	305	UFT	C4-N3-C2	-5.01	119.97	126.58
1	B	577	UFT	C4-N3-C2	-5.01	119.97	126.58
1	A	653	UFT	C4-N3-C2	-5.01	119.97	126.58
1	B	169	UFT	C4-N3-C2	-5.01	119.98	126.58
1	B	347	UFT	C4-N3-C2	-5.01	119.98	126.58
1	A	635	UFT	C4-N3-C2	-5.01	119.98	126.58
1	A	60	UFT	C4-N3-C2	-5.01	119.98	126.58
1	A	208	UFT	C4-N3-C2	-5.01	119.98	126.58
1	B	214	UFT	C4-N3-C2	-5.01	119.98	126.58
1	A	471	UFT	C4-N3-C2	-5.01	119.98	126.58
1	B	695	UFT	C4-N3-C2	-5.00	119.98	126.58
1	A	169	UFT	C4-N3-C2	-5.00	119.98	126.58
1	A	182	UFT	C4-N3-C2	-5.00	119.98	126.58
1	A	607	UFT	C4-N3-C2	-5.00	119.98	126.58
1	A	266	UFT	C4-N3-C2	-5.00	119.98	126.58
1	B	266	UFT	C4-N3-C2	-5.00	119.98	126.58
1	A	559	UFT	C4-N3-C2	-5.00	119.99	126.58
1	A	590	UFT	C4-N3-C2	-5.00	119.99	126.58
1	B	621	UFT	C4-N3-C2	-5.00	119.99	126.58
1	A	689	UFT	C4-N3-C2	-5.00	119.99	126.58
1	B	69	UFT	C4-N3-C2	-5.00	119.99	126.58
1	B	97	UFT	C4-N3-C2	-5.00	119.99	126.58
1	A	366	UFT	C4-N3-C2	-5.00	119.99	126.58
1	A	59	UFT	C4-N3-C2	-5.00	119.99	126.58
1	B	471	UFT	C4-N3-C2	-5.00	119.99	126.58
1	B	365	UFT	C4-N3-C2	-4.99	119.99	126.58
1	B	423	UFT	C4-N3-C2	-4.99	119.99	126.58
1	A	434	UFT	C4-N3-C2	-4.99	119.99	126.58
1	A	447	UFT	C4-N3-C2	-4.99	119.99	126.58
1	B	251	UFT	C4-N3-C2	-4.99	120.00	126.58
1	A	97	UFT	C4-N3-C2	-4.99	120.00	126.58
1	B	208	UFT	C4-N3-C2	-4.99	120.00	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	UFT	C4-N3-C2	-4.99	120.00	126.58
1	B	71	UFT	C4-N3-C2	-4.99	120.00	126.58
1	B	366	UFT	C4-N3-C2	-4.99	120.00	126.58
1	A	695	UFT	C4-N3-C2	-4.99	120.00	126.58
1	A	618	UFT	C4-N3-C2	-4.99	120.00	126.58
1	A	593	UFT	C4-N3-C2	-4.99	120.00	126.58
1	A	545	UFT	C4-N3-C2	-4.99	120.00	126.58
1	B	309	UFT	C4-N3-C2	-4.99	120.00	126.58
1	A	719	UFT	C4-N3-C2	-4.98	120.00	126.58
1	A	485	UFT	C4-N3-C2	-4.98	120.01	126.58
1	B	607	UFT	C4-N3-C2	-4.98	120.01	126.58
1	B	437	UFT	C4-N3-C2	-4.98	120.01	126.58
1	B	456	UFT	C4-N3-C2	-4.98	120.01	126.58
1	B	55	UFT	C4-N3-C2	-4.98	120.01	126.58
1	A	708	UFT	C4-N3-C2	-4.98	120.01	126.58
1	B	628	UFT	C4-N3-C2	-4.98	120.01	126.58
1	B	137	UFT	C4-N3-C2	-4.98	120.02	126.58
1	A	50	UFT	C4-N3-C2	-4.98	120.02	126.58
1	A	106	UFT	C4-N3-C2	-4.98	120.02	126.58
1	B	153	UFT	C4-N3-C2	-4.98	120.02	126.58
1	A	628	UFT	C4-N3-C2	-4.98	120.02	126.58
1	B	344	UFT	C4-N3-C2	-4.98	120.02	126.58
1	A	112	UFT	C4-N3-C2	-4.97	120.02	126.58
1	B	701	UFT	C4-N3-C2	-4.97	120.02	126.58
1	B	646	UFT	C4-N3-C2	-4.97	120.02	126.58
1	B	555	UFT	C4-N3-C2	-4.97	120.02	126.58
1	B	545	UFT	C4-N3-C2	-4.97	120.02	126.58
1	A	8	UFT	C4-N3-C2	-4.97	120.03	126.58
1	A	55	UFT	C4-N3-C2	-4.97	120.03	126.58
1	B	581	UFT	C4-N3-C2	-4.97	120.03	126.58
1	B	305	UFT	C4-N3-C2	-4.97	120.03	126.58
1	B	590	UFT	C4-N3-C2	-4.97	120.03	126.58
1	A	44	UFT	C4-N3-C2	-4.97	120.03	126.58
1	A	153	UFT	C4-N3-C2	-4.97	120.03	126.58
1	A	251	UFT	C4-N3-C2	-4.97	120.03	126.58
1	A	423	UFT	C4-N3-C2	-4.97	120.03	126.58
1	B	534	UFT	C4-N3-C2	-4.97	120.03	126.58
1	A	98	UFT	C4-N3-C2	-4.96	120.03	126.58
1	A	48	UFT	C4-N3-C2	-4.96	120.03	126.58
1	B	229	UFT	C4-N3-C2	-4.96	120.03	126.58
1	A	309	UFT	C4-N3-C2	-4.96	120.03	126.58
1	B	447	UFT	C4-N3-C2	-4.96	120.03	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	UFT	C4-N3-C2	-4.96	120.03	126.58
1	A	571	UFT	C4-N3-C2	-4.96	120.03	126.58
1	A	581	UFT	C4-N3-C2	-4.96	120.03	126.58
1	B	559	UFT	C4-N3-C2	-4.96	120.03	126.58
1	B	571	UFT	C4-N3-C2	-4.96	120.03	126.58
1	A	179	UFT	C4-N3-C2	-4.96	120.04	126.58
1	A	456	UFT	C4-N3-C2	-4.96	120.04	126.58
1	B	502	UFT	C4-N3-C2	-4.96	120.04	126.58
1	B	179	UFT	C4-N3-C2	-4.96	120.04	126.58
1	A	629	UFT	C4-N3-C2	-4.96	120.04	126.58
1	A	94	UFT	C4-N3-C2	-4.96	120.04	126.58
1	A	503	UFT	C4-N3-C2	-4.96	120.04	126.58
1	B	708	UFT	C4-N3-C2	-4.96	120.04	126.58
1	B	163	UFT	C4-N3-C2	-4.96	120.04	126.58
1	A	549	UFT	C4-N3-C2	-4.96	120.04	126.58
1	A	365	UFT	C4-N3-C2	-4.95	120.05	126.58
1	A	367	UFT	C4-N3-C2	-4.95	120.05	126.58
1	B	509	UFT	C4-N3-C2	-4.95	120.05	126.58
1	A	701	UFT	C4-N3-C2	-4.95	120.05	126.58
1	B	8	UFT	C4-N3-C2	-4.95	120.05	126.58
1	B	629	UFT	C4-N3-C2	-4.95	120.05	126.58
1	A	260	UFT	C4-N3-C2	-4.95	120.05	126.58
1	A	141	UFT	C4-N3-C2	-4.95	120.05	126.58
1	B	260	UFT	C4-N3-C2	-4.95	120.05	126.58
1	B	389	UFT	C4-N3-C2	-4.95	120.06	126.58
1	A	84	UFT	C4-N3-C2	-4.94	120.06	126.58
1	A	329	UFT	C4-N3-C2	-4.94	120.06	126.58
1	A	712	UFT	C4-N3-C2	-4.94	120.06	126.58
1	B	33	UFT	C4-N3-C2	-4.94	120.06	126.58
1	A	108	UFT	C4-N3-C2	-4.94	120.06	126.58
1	A	163	UFT	C4-N3-C2	-4.94	120.06	126.58
1	A	509	UFT	C4-N3-C2	-4.94	120.06	126.58
1	B	712	UFT	C4-N3-C2	-4.94	120.06	126.58
1	A	687	UFT	C4-N3-C2	-4.94	120.06	126.58
1	A	71	UFT	C4-N3-C2	-4.94	120.07	126.58
1	B	656	UFT	C4-N3-C2	-4.94	120.07	126.58
1	B	141	UFT	C4-N3-C2	-4.94	120.07	126.58
1	A	334	UFT	C4-N3-C2	-4.94	120.07	126.58
1	B	32	UFT	C4-N3-C2	-4.94	120.07	126.58
1	A	402	UFT	C4-N3-C2	-4.94	120.07	126.58
1	A	302	UFT	C4-N3-C2	-4.94	120.07	126.58
1	A	534	UFT	C4-N3-C2	-4.94	120.07	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	UFT	C4-N3-C2	-4.93	120.07	126.58
1	B	108	UFT	C4-N3-C2	-4.93	120.07	126.58
1	B	334	UFT	C4-N3-C2	-4.93	120.07	126.58
1	A	602	UFT	C4-N3-C2	-4.93	120.08	126.58
1	A	472	UFT	C4-N3-C2	-4.93	120.08	126.58
1	B	106	UFT	C4-N3-C2	-4.93	120.08	126.58
1	B	175	UFT	C4-N3-C2	-4.93	120.08	126.58
1	B	673	UFT	C4-N3-C2	-4.93	120.08	126.58
1	B	84	UFT	C4-N3-C2	-4.93	120.08	126.58
1	B	687	UFT	C4-N3-C2	-4.93	120.08	126.58
1	B	719	UFT	C4-N3-C2	-4.93	120.08	126.58
1	B	549	UFT	C4-N3-C2	-4.92	120.08	126.58
1	B	402	UFT	C4-N3-C2	-4.92	120.09	126.58
1	B	204	UFT	C4-N3-C2	-4.92	120.09	126.58
1	A	192	UFT	C4-N3-C2	-4.92	120.09	126.58
1	B	302	UFT	C4-N3-C2	-4.91	120.10	126.58
1	B	432	UFT	C4-N3-C2	-4.91	120.10	126.58
1	A	502	UFT	C4-N3-C2	-4.91	120.10	126.58
1	A	344	UFT	C4-N3-C2	-4.91	120.10	126.58
1	B	50	UFT	C4-N3-C2	-4.91	120.10	126.58
1	A	421	UFT	C4-N3-C2	-4.91	120.10	126.58
1	A	313	UFT	C4-N3-C2	-4.91	120.11	126.58
1	B	352	UFT	C4-N3-C2	-4.90	120.11	126.58
1	A	233	UFT	C4-N3-C2	-4.90	120.11	126.58
1	B	421	UFT	C4-N3-C2	-4.90	120.11	126.58
1	B	80	UFT	C4-N3-C2	-4.90	120.12	126.58
1	B	174	UFT	C4-N3-C2	-4.89	120.12	126.58
1	A	656	UFT	C4-N3-C2	-4.89	120.12	126.58
1	A	174	UFT	C4-N3-C2	-4.89	120.13	126.58
1	B	60	UFT	C4-N3-C2	-4.89	120.13	126.58
1	B	602	UFT	C4-N3-C2	-4.89	120.13	126.58
1	A	703	UFT	C4-N3-C2	-4.89	120.13	126.58
1	A	175	UFT	C4-N3-C2	-4.89	120.13	126.58
1	B	192	UFT	C4-N3-C2	-4.89	120.13	126.58
1	A	214	UFT	C4-N3-C2	-4.89	120.13	126.58
1	A	229	UFT	C4-N3-C2	-4.89	120.13	126.58
1	B	524	UFT	C4-N3-C2	-4.88	120.14	126.58
1	A	293	UFT	C4-N3-C2	-4.88	120.14	126.58
1	B	233	UFT	C4-N3-C2	-4.88	120.14	126.58
1	B	485	UFT	C4-N3-C2	-4.88	120.14	126.58
1	A	499	UFT	C4-N3-C2	-4.88	120.14	126.58
1	B	245	UFT	C4-N3-C2	-4.88	120.15	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	UFT	C4-N3-C2	-4.88	120.15	126.58
1	A	432	UFT	C4-N3-C2	-4.87	120.15	126.58
1	A	460	UFT	C4-N3-C2	-4.87	120.15	126.58
1	B	59	UFT	C4-N3-C2	-4.87	120.16	126.58
1	B	720	UFT	C4-N3-C2	-4.87	120.16	126.58
1	A	673	UFT	C4-N3-C2	-4.87	120.16	126.58
1	A	684	UFT	C4-N3-C2	-4.87	120.16	126.58
1	B	460	UFT	C4-N3-C2	-4.86	120.17	126.58
1	A	11	UFT	C4-N3-C2	-4.86	120.17	126.58
1	A	135	UFT	C4-N3-C2	-4.86	120.17	126.58
1	A	544	UFT	C4-N3-C2	-4.85	120.18	126.58
1	A	92	UFT	C4-N3-C2	-4.85	120.18	126.58
1	B	544	UFT	C4-N3-C2	-4.85	120.18	126.58
1	B	669	UFT	C4-N3-C2	-4.85	120.18	126.58
1	B	92	UFT	C4-N3-C2	-4.85	120.19	126.58
1	A	196	UFT	C4-N3-C2	-4.85	120.19	126.58
1	A	361	UFT	C4-N3-C2	-4.84	120.19	126.58
1	A	389	UFT	C4-N3-C2	-4.84	120.19	126.58
1	B	499	UFT	C4-N3-C2	-4.84	120.19	126.58
1	B	472	UFT	C4-N3-C2	-4.84	120.20	126.58
1	B	196	UFT	C4-N3-C2	-4.84	120.20	126.58
1	A	322	UFT	C4-N3-C2	-4.84	120.20	126.58
1	A	413	UFT	C4-N3-C2	-4.83	120.20	126.58
1	A	33	UFT	C4-N3-C2	-4.83	120.21	126.58
1	A	464	UFT	C4-N3-C2	-4.83	120.21	126.58
1	A	215	UFT	C4-N3-C2	-4.82	120.22	126.58
1	A	377	UFT	C4-N3-C2	-4.82	120.22	126.58
1	B	684	UFT	C4-N3-C2	-4.82	120.22	126.58
1	B	464	UFT	C4-N3-C2	-4.82	120.22	126.58
1	B	703	UFT	C4-N3-C2	-4.82	120.22	126.58
1	A	80	UFT	C4-N3-C2	-4.81	120.23	126.58
1	A	669	UFT	C4-N3-C2	-4.81	120.23	126.58
1	A	513	UFT	C4-N3-C2	-4.80	120.25	126.58
1	B	513	UFT	C4-N3-C2	-4.80	120.25	126.58
1	A	530	UFT	C4-N3-C2	-4.80	120.25	126.58
1	B	377	UFT	C4-N3-C2	-4.79	120.26	126.58
1	A	42	UFT	C4-N3-C2	-4.79	120.27	126.58
1	B	135	UFT	C4-N3-C2	-4.78	120.28	126.58
1	B	481	UFT	C4-N3-C2	-4.77	120.29	126.58
1	A	524	UFT	C4-N3-C2	-4.75	120.31	126.58
1	B	676	UFT	C4-N3-C2	-4.73	120.34	126.58
1	A	358	UFT	C4-N3-C2	-4.73	120.35	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	UFT	C4-N3-C2	-4.72	120.35	126.58
1	A	481	UFT	C4-N3-C2	-4.72	120.35	126.58
1	A	676	UFT	C4-N3-C2	-4.71	120.36	126.58
1	A	105	UFT	C4-N3-C2	-4.71	120.37	126.58
1	B	535	UFT	C4-N3-C2	-4.69	120.40	126.58
1	B	216	UFT	C4-N3-C2	-4.68	120.41	126.58
1	B	358	UFT	C4-N3-C2	-4.67	120.42	126.58
1	B	489	UFT	C4-N3-C2	-4.66	120.43	126.58
1	B	105	UFT	C4-N3-C2	-4.63	120.47	126.58
1	A	535	UFT	C4-N3-C2	-4.62	120.49	126.58
1	B	42	UFT	C4-N3-C2	-4.61	120.50	126.58
1	A	659	UFT	C4-N3-C2	-4.60	120.51	126.58
1	B	659	UFT	C4-N3-C2	-4.60	120.51	126.58
1	B	43	UFT	C4-N3-C2	-4.59	120.53	126.58
1	A	43	UFT	C4-N3-C2	-4.58	120.54	126.58
1	A	359	UFT	C4-N3-C2	-4.49	120.66	126.58
1	A	517	CFZ	C3'-C2'-C1'	4.43	108.49	103.13
1	B	25	CFZ	C2'-C3'-C4'	4.36	108.04	102.40
1	A	536	CFZ	C3'-C2'-C1'	4.35	108.39	103.13
1	A	606	UFT	C2'-C3'-C4'	4.30	107.96	102.40
1	B	241	CFZ	C2'-C3'-C4'	4.30	107.95	102.40
1	A	241	CFZ	C2'-C3'-C4'	4.26	107.91	102.40
1	B	493	UFT	C4-N3-C2	-4.24	120.99	126.58
1	B	417	CFZ	C2'-C3'-C4'	4.21	107.85	102.40
1	A	241	CFZ	C3'-C2'-C1'	4.20	108.22	103.13
1	B	241	CFZ	C3'-C2'-C1'	4.20	108.22	103.13
1	B	439	CFZ	C2'-C3'-C4'	4.20	107.83	102.40
1	A	417	CFZ	C2'-C3'-C4'	4.19	107.82	102.40
1	B	720	UFT	N3-C2-N1	4.17	120.43	114.89
1	B	362	CFZ	C3'-C2'-C1'	4.17	108.18	103.13
1	A	13	UFT	C2'-C3'-C4'	4.17	107.79	102.40
1	A	664	CFZ	C2'-C3'-C4'	4.16	107.78	102.40
1	A	439	CFZ	C3'-C2'-C1'	4.16	108.17	103.13
1	B	446	CFZ	C2'-C3'-C4'	4.16	107.78	102.40
1	B	361	UFT	C3'-C2'-C1'	4.15	108.16	103.13
1	A	144	CFZ	C2'-C3'-C4'	4.15	107.76	102.40
1	B	144	CFZ	C2'-C3'-C4'	4.15	107.76	102.40
1	B	664	CFZ	C2'-C3'-C4'	4.14	107.76	102.40
1	B	321	CFZ	C2'-C3'-C4'	4.14	107.75	102.40
1	A	14	UFT	N3-C2-N1	4.14	120.38	114.89
1	A	655	CFZ	C3'-C2'-C1'	4.14	108.14	103.13
1	A	517	CFZ	C2'-C3'-C4'	4.13	107.75	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	CFZ	C2'-C3'-C4'	4.13	107.74	102.40
1	B	308	CFZ	C2'-C3'-C4'	4.13	107.74	102.40
1	A	719	UFT	C2'-C3'-C4'	4.13	107.74	102.40
1	B	536	CFZ	C3'-C2'-C1'	4.11	108.11	103.13
1	B	655	CFZ	C3'-C2'-C1'	4.11	108.11	103.13
1	A	353	CFZ	C2'-C3'-C4'	4.11	107.71	102.40
1	B	664	CFZ	C3'-C2'-C1'	4.11	108.10	103.13
1	B	338	CFZ	C3'-C2'-C1'	4.10	108.09	103.13
1	A	214	UFT	N3-C2-N1	4.09	120.32	114.89
1	A	268	CFZ	C3'-C2'-C1'	4.08	108.08	103.13
1	B	13	UFT	C2'-C3'-C4'	4.08	107.67	102.40
1	B	90	CFZ	C3'-C2'-C1'	4.07	108.06	103.13
1	B	308	CFZ	C3'-C2'-C1'	4.07	108.06	103.13
1	B	28	CFZ	C4'-O4'-C1'	-4.07	100.49	109.47
1	A	664	CFZ	C3'-C2'-C1'	4.07	108.06	103.13
1	B	171	CFZ	C2'-C3'-C4'	4.07	107.66	102.40
1	B	171	CFZ	C3'-C2'-C1'	4.07	108.06	103.13
1	B	144	CFZ	C3'-C2'-C1'	4.07	108.05	103.13
1	A	328	CFZ	C3'-C2'-C1'	4.06	108.04	103.13
1	A	75	CFZ	C2'-C3'-C4'	4.05	107.64	102.40
1	A	144	CFZ	C3'-C2'-C1'	4.05	108.03	103.13
1	A	90	CFZ	C2'-C3'-C4'	4.05	107.63	102.40
1	A	308	CFZ	C2'-C3'-C4'	4.04	107.62	102.40
1	B	673	UFT	C2'-C3'-C4'	4.04	107.62	102.40
1	A	19	UFT	N3-C2-N1	4.04	120.25	114.89
1	A	215	UFT	N3-C2-N1	4.04	120.25	114.89
1	A	440	CFZ	C2'-C3'-C4'	4.04	107.62	102.40
1	A	171	CFZ	C2'-C3'-C4'	4.03	107.61	102.40
1	B	472	UFT	C3'-C2'-C1'	4.03	108.01	103.13
1	A	117	CFZ	C3'-C2'-C1'	4.03	108.00	103.13
1	A	308	CFZ	C3'-C2'-C1'	4.03	108.00	103.13
1	A	673	UFT	C2'-C3'-C4'	4.03	107.61	102.40
1	B	361	UFT	C2'-C3'-C4'	4.02	107.60	102.40
1	A	171	CFZ	C3'-C2'-C1'	4.02	108.00	103.13
1	B	362	CFZ	C2'-C3'-C4'	4.01	107.58	102.40
1	B	485	UFT	C2'-C3'-C4'	4.00	107.58	102.40
1	B	536	CFZ	C2'-C3'-C4'	4.00	107.57	102.40
1	A	105	UFT	C3'-C2'-C1'	3.99	107.96	103.13
1	B	63	CFZ	C3'-C2'-C1'	3.99	107.96	103.13
1	A	328	CFZ	C2'-C3'-C4'	3.99	107.56	102.40
1	B	19	UFT	N3-C2-N1	3.98	120.18	114.89
1	A	117	CFZ	C2'-C3'-C4'	3.98	107.55	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	CFZ	C2'-C3'-C4'	3.98	107.55	102.40
1	B	117	CFZ	C3'-C2'-C1'	3.98	107.94	103.13
1	A	283	UFT	N3-C2-N1	3.98	120.17	114.89
1	A	200	UFT	C2'-C3'-C4'	3.97	107.54	102.40
1	B	105	UFT	C3'-C2'-C1'	3.97	107.94	103.13
1	B	432	UFT	C2'-C1'-N1	-3.97	108.14	114.20
1	B	14	UFT	N3-C2-N1	3.96	120.15	114.89
1	A	32	UFT	N3-C2-N1	3.96	120.14	114.89
1	B	283	UFT	N3-C2-N1	3.96	120.14	114.89
1	B	637	CFZ	C3'-C2'-C1'	3.96	107.92	103.13
1	B	25	CFZ	C3'-C2'-C1'	3.95	107.92	103.13
1	A	583	CFZ	C3'-C2'-C1'	3.95	107.91	103.13
1	A	90	CFZ	C3'-C2'-C1'	3.95	107.91	103.13
1	B	11	UFT	N3-C2-N1	3.95	120.13	114.89
1	B	583	CFZ	C3'-C2'-C1'	3.95	107.91	103.13
1	B	577	UFT	N3-C2-N1	3.95	120.13	114.89
1	B	633	UFT	N3-C2-N1	3.95	120.13	114.89
1	B	117	CFZ	C2'-C3'-C4'	3.95	107.50	102.40
1	B	606	UFT	C2'-C3'-C4'	3.95	107.50	102.40
1	B	245	UFT	N3-C2-N1	3.94	120.12	114.89
1	A	63	CFZ	C2'-C3'-C4'	3.94	107.49	102.40
1	B	8	UFT	C3'-C2'-C1'	3.94	107.90	103.13
1	A	63	CFZ	C3'-C2'-C1'	3.94	107.90	103.13
1	B	301	UFT	N3-C2-N1	3.94	120.12	114.89
1	B	431	UFT	N3-C2-N1	3.94	120.12	114.89
1	A	633	UFT	N3-C2-N1	3.94	120.12	114.89
1	A	637	CFZ	C3'-C2'-C1'	3.93	107.89	103.13
1	B	90	CFZ	C2'-C3'-C4'	3.93	107.48	102.40
1	B	170	UFT	C2'-C3'-C4'	3.93	107.48	102.40
1	A	417	CFZ	C3'-C2'-C1'	3.93	107.89	103.13
1	B	60	UFT	C2'-C3'-C4'	3.93	107.48	102.40
1	B	13	UFT	N3-C2-N1	3.93	120.10	114.89
1	A	607	UFT	N3-C2-N1	3.93	120.10	114.89
1	B	502	UFT	C2'-C3'-C4'	3.93	107.47	102.40
1	B	629	UFT	N3-C2-N1	3.92	120.10	114.89
1	B	48	UFT	N3-C2-N1	3.92	120.10	114.89
1	A	190	UFT	N3-C2-N1	3.92	120.10	114.89
1	A	251	UFT	N3-C2-N1	3.92	120.10	114.89
1	A	347	UFT	N3-C2-N1	3.92	120.10	114.89
1	A	519	UFT	N3-C2-N1	3.92	120.10	114.89
1	A	13	UFT	N3-C2-N1	3.92	120.10	114.89
1	B	67	CFZ	C3'-C2'-C1'	3.92	107.88	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	629	UFT	N3-C2-N1	3.92	120.09	114.89
1	B	50	UFT	C3'-C2'-C1'	3.92	107.88	103.13
1	A	108	UFT	N3-C2-N1	3.92	120.09	114.89
1	B	666	UFT	N3-C2-N1	3.92	120.09	114.89
1	B	347	UFT	N3-C2-N1	3.92	120.09	114.89
1	A	268	CFZ	C2'-C3'-C4'	3.92	107.46	102.40
1	B	606	UFT	N3-C2-N1	3.92	120.09	114.89
1	B	268	CFZ	C3'-C2'-C1'	3.91	107.87	103.13
1	B	504	UFT	N3-C2-N1	3.91	120.08	114.89
1	B	251	UFT	N3-C2-N1	3.91	120.08	114.89
1	A	524	UFT	N3-C2-N1	3.91	120.08	114.89
1	A	439	CFZ	C2'-C3'-C4'	3.91	107.46	102.40
1	B	328	CFZ	C3'-C2'-C1'	3.91	107.86	103.13
1	B	86	UFT	N3-C2-N1	3.91	120.08	114.89
1	A	438	CFZ	C3'-C2'-C1'	3.91	107.86	103.13
1	B	170	UFT	C3'-C2'-C1'	3.91	107.86	103.13
1	A	367	UFT	N3-C2-N1	3.91	120.08	114.89
1	B	690	UFT	N3-C2-N1	3.91	120.08	114.89
1	A	655	CFZ	C2'-C3'-C4'	3.91	107.45	102.40
1	A	137	UFT	N3-C2-N1	3.90	120.07	114.89
1	B	472	UFT	C2'-C3'-C4'	3.90	107.44	102.40
1	B	367	UFT	N3-C2-N1	3.90	120.07	114.89
1	A	403	UFT	N3-C2-N1	3.90	120.07	114.89
1	B	313	UFT	N3-C2-N1	3.90	120.07	114.89
1	A	577	UFT	N3-C2-N1	3.90	120.07	114.89
1	B	359	UFT	N3-C2-N1	3.90	120.07	114.89
1	A	200	UFT	N3-C2-N1	3.90	120.06	114.89
1	B	437	UFT	N3-C2-N1	3.90	120.06	114.89
1	B	108	UFT	N3-C2-N1	3.90	120.06	114.89
1	B	112	UFT	N3-C2-N1	3.90	120.06	114.89
1	B	336	UFT	N3-C2-N1	3.89	120.06	114.89
1	A	690	UFT	N3-C2-N1	3.89	120.06	114.89
1	B	143	UFT	C3'-C2'-C1'	3.89	107.85	103.13
1	B	628	UFT	N3-C2-N1	3.89	120.06	114.89
1	A	69	UFT	N3-C2-N1	3.89	120.06	114.89
1	B	329	UFT	N3-C2-N1	3.89	120.06	114.89
1	B	663	UFT	C3'-C2'-C1'	3.89	107.84	103.13
1	A	86	UFT	N3-C2-N1	3.89	120.06	114.89
1	B	217	UFT	N3-C2-N1	3.89	120.06	114.89
1	A	437	UFT	N3-C2-N1	3.89	120.06	114.89
1	A	646	UFT	N3-C2-N1	3.89	120.06	114.89
1	B	202	UFT	N3-C2-N1	3.89	120.05	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	UFT	N3-C2-N1	3.89	120.05	114.89
1	A	301	UFT	N3-C2-N1	3.89	120.05	114.89
1	B	163	UFT	N3-C2-N1	3.89	120.05	114.89
1	B	646	UFT	N3-C2-N1	3.89	120.05	114.89
1	A	666	UFT	N3-C2-N1	3.89	120.05	114.89
1	A	170	UFT	C3'-C2'-C1'	3.89	107.84	103.13
1	B	137	UFT	N3-C2-N1	3.89	120.05	114.89
1	B	215	UFT	N3-C2-N1	3.89	120.05	114.89
1	A	143	UFT	C3'-C2'-C1'	3.89	107.84	103.13
1	A	115	UFT	N3-C2-N1	3.89	120.05	114.89
1	B	160	UFT	N3-C2-N1	3.89	120.05	114.89
1	A	202	UFT	N3-C2-N1	3.89	120.05	114.89
1	B	434	UFT	N3-C2-N1	3.89	120.05	114.89
1	A	160	UFT	N3-C2-N1	3.89	120.05	114.89
1	B	214	UFT	N3-C2-N1	3.88	120.05	114.89
1	B	96	CFZ	C3'-C2'-C1'	3.88	107.83	103.13
1	B	471	UFT	N3-C2-N1	3.88	120.05	114.89
1	B	554	UFT	N3-C2-N1	3.88	120.05	114.89
1	B	417	CFZ	C3'-C2'-C1'	3.88	107.83	103.13
1	A	431	UFT	N3-C2-N1	3.88	120.04	114.89
1	A	663	UFT	C3'-C2'-C1'	3.88	107.83	103.13
1	A	179	UFT	N3-C2-N1	3.88	120.04	114.89
1	B	114	CFZ	C2'-C3'-C4'	3.88	107.42	102.40
1	A	170	UFT	N3-C2-N1	3.88	120.04	114.89
1	A	270	UFT	N3-C2-N1	3.88	120.04	114.89
1	B	608	UFT	N3-C2-N1	3.88	120.04	114.89
1	B	62	UFT	N3-C2-N1	3.88	120.04	114.89
1	A	606	UFT	N3-C2-N1	3.88	120.04	114.89
1	A	353	CFZ	C3'-C2'-C1'	3.88	107.83	103.13
1	B	43	UFT	C2'-C3'-C4'	3.88	107.42	102.40
1	B	608	UFT	C2'-C3'-C4'	3.88	107.42	102.40
1	B	190	UFT	N3-C2-N1	3.88	120.04	114.89
1	A	336	UFT	N3-C2-N1	3.88	120.04	114.89
1	B	493	UFT	N3-C2-N1	3.88	120.04	114.89
1	B	115	UFT	N3-C2-N1	3.88	120.04	114.89
1	B	530	UFT	N3-C2-N1	3.88	120.04	114.89
1	A	112	UFT	N3-C2-N1	3.88	120.04	114.89
1	A	154	UFT	N3-C2-N1	3.88	120.04	114.89
1	A	504	UFT	N3-C2-N1	3.88	120.04	114.89
1	A	486	CFZ	C2'-C1'-N1	-3.88	108.28	114.20
1	A	444	CFZ	C3'-C2'-C1'	3.88	107.82	103.13
1	B	197	UFT	N3-C2-N1	3.88	120.03	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	534	UFT	N3-C2-N1	3.88	120.03	114.89
1	A	590	UFT	N3-C2-N1	3.88	120.03	114.89
1	B	116	UFT	N3-C2-N1	3.88	120.03	114.89
1	A	142	UFT	N3-C2-N1	3.88	120.03	114.89
1	B	296	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	447	UFT	N3-C2-N1	3.87	120.03	114.89
1	B	593	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	502	UFT	C2'-C3'-C4'	3.87	107.41	102.40
1	A	101	UFT	N3-C2-N1	3.87	120.03	114.89
1	B	403	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	554	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	720	UFT	N3-C2-N1	3.87	120.03	114.89
1	B	88	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	126	UFT	N3-C2-N1	3.87	120.03	114.89
1	B	266	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	362	CFZ	C3'-C2'-C1'	3.87	107.82	103.13
1	B	63	CFZ	C2'-C3'-C4'	3.87	107.41	102.40
1	A	61	UFT	N3-C2-N1	3.87	120.03	114.89
1	B	590	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	609	UFT	N3-C2-N1	3.87	120.03	114.89
1	B	653	UFT	N3-C2-N1	3.87	120.03	114.89
1	B	662	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	673	UFT	C3'-C2'-C1'	3.87	107.82	103.13
1	B	101	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	106	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	208	UFT	N3-C2-N1	3.87	120.03	114.89
1	B	696	UFT	N3-C2-N1	3.87	120.03	114.89
1	B	719	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	8	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	696	UFT	N3-C2-N1	3.87	120.03	114.89
1	A	75	CFZ	C3'-C2'-C1'	3.87	107.81	103.13
1	A	74	UFT	N3-C2-N1	3.87	120.03	114.89
1	B	94	UFT	N3-C2-N1	3.87	120.02	114.89
1	B	582	UFT	N3-C2-N1	3.87	120.02	114.89
1	A	662	UFT	N3-C2-N1	3.87	120.02	114.89
1	B	689	UFT	N3-C2-N1	3.87	120.02	114.89
1	A	663	UFT	N3-C2-N1	3.87	120.02	114.89
1	A	719	UFT	C3'-C2'-C1'	3.87	107.81	103.13
1	B	637	CFZ	C2'-C3'-C4'	3.87	107.40	102.40
1	A	266	UFT	N3-C2-N1	3.87	120.02	114.89
1	B	126	UFT	N3-C2-N1	3.87	120.02	114.89
1	A	582	UFT	N3-C2-N1	3.87	120.02	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	CFZ	C3'-C2'-C1'	3.86	107.81	103.13
1	B	142	UFT	N3-C2-N1	3.86	120.02	114.89
1	A	430	UFT	N3-C2-N1	3.86	120.02	114.89
1	A	545	UFT	N3-C2-N1	3.86	120.02	114.89
1	A	637	CFZ	C2'-C3'-C4'	3.86	107.40	102.40
1	B	609	UFT	N3-C2-N1	3.86	120.02	114.89
1	A	170	UFT	C2'-C3'-C4'	3.86	107.39	102.40
1	B	365	UFT	N3-C2-N1	3.86	120.02	114.89
1	B	61	UFT	N3-C2-N1	3.86	120.02	114.89
1	B	170	UFT	N3-C2-N1	3.86	120.02	114.89
1	A	542	UFT	N3-C2-N1	3.86	120.02	114.89
1	A	536	CFZ	C2'-C3'-C4'	3.86	107.39	102.40
1	B	32	UFT	N3-C2-N1	3.86	120.02	114.89
1	B	200	UFT	N3-C2-N1	3.86	120.02	114.89
1	A	628	UFT	N3-C2-N1	3.86	120.02	114.89
1	A	94	UFT	N3-C2-N1	3.86	120.02	114.89
1	B	366	UFT	N3-C2-N1	3.86	120.02	114.89
1	B	344	UFT	N3-C2-N1	3.86	120.01	114.89
1	B	466	UFT	N3-C2-N1	3.86	120.01	114.89
1	B	50	UFT	C2'-C3'-C4'	3.86	107.39	102.40
1	A	282	CFZ	C2'-C3'-C4'	3.86	107.39	102.40
1	A	366	UFT	N3-C2-N1	3.86	120.01	114.89
1	B	502	UFT	N3-C2-N1	3.86	120.01	114.89
1	A	59	UFT	N3-C2-N1	3.86	120.01	114.89
1	A	555	UFT	N3-C2-N1	3.86	120.01	114.89
1	B	358	UFT	N3-C2-N1	3.86	120.01	114.89
1	A	329	UFT	N3-C2-N1	3.86	120.01	114.89
1	B	500	UFT	N3-C2-N1	3.86	120.01	114.89
1	A	116	UFT	N3-C2-N1	3.86	120.01	114.89
1	A	296	UFT	N3-C2-N1	3.86	120.01	114.89
1	A	471	UFT	N3-C2-N1	3.86	120.01	114.89
1	B	545	UFT	N3-C2-N1	3.86	120.01	114.89
1	A	636	UFT	N3-C2-N1	3.86	120.01	114.89
1	A	689	UFT	N3-C2-N1	3.85	120.01	114.89
1	B	143	UFT	N3-C2-N1	3.85	120.01	114.89
1	B	208	UFT	N3-C2-N1	3.85	120.01	114.89
1	A	143	UFT	N3-C2-N1	3.85	120.00	114.89
1	A	155	UFT	N3-C2-N1	3.85	120.00	114.89
1	A	169	UFT	N3-C2-N1	3.85	120.00	114.89
1	B	695	UFT	N3-C2-N1	3.85	120.00	114.89
1	B	33	UFT	N3-C2-N1	3.85	120.00	114.89
1	A	88	UFT	N3-C2-N1	3.85	120.00	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	UFT	N3-C2-N1	3.85	120.00	114.89
1	B	97	UFT	N3-C2-N1	3.85	120.00	114.89
1	A	593	UFT	N3-C2-N1	3.85	120.00	114.89
1	B	583	CFZ	C2'-C3'-C4'	3.85	107.38	102.40
1	B	169	UFT	N3-C2-N1	3.85	120.00	114.89
1	B	182	UFT	N3-C2-N1	3.85	120.00	114.89
1	A	141	UFT	N3-C2-N1	3.85	120.00	114.89
1	B	421	UFT	N3-C2-N1	3.85	120.00	114.89
1	B	542	UFT	N3-C2-N1	3.85	120.00	114.89
1	A	636	UFT	C3'-C2'-C1'	3.85	107.79	103.13
1	B	155	UFT	N3-C2-N1	3.85	120.00	114.89
1	A	344	UFT	N3-C2-N1	3.85	120.00	114.89
1	B	456	UFT	N3-C2-N1	3.85	120.00	114.89
1	B	509	UFT	N3-C2-N1	3.85	120.00	114.89
1	A	708	UFT	N3-C2-N1	3.85	120.00	114.89
1	A	503	UFT	N3-C2-N1	3.85	120.00	114.89
1	A	48	UFT	C2'-C3'-C4'	3.85	107.37	102.40
1	B	154	UFT	N3-C2-N1	3.85	119.99	114.89
1	A	719	UFT	N3-C2-N1	3.85	119.99	114.89
1	B	179	UFT	N3-C2-N1	3.84	119.99	114.89
1	A	653	UFT	N3-C2-N1	3.84	119.99	114.89
1	B	438	CFZ	C3'-C2'-C1'	3.84	107.78	103.13
1	B	50	UFT	N3-C2-N1	3.84	119.99	114.89
1	A	55	UFT	N3-C2-N1	3.84	119.99	114.89
1	A	398	UFT	N3-C2-N1	3.84	119.99	114.89
1	B	708	UFT	N3-C2-N1	3.84	119.99	114.89
1	A	265	UFT	N3-C2-N1	3.84	119.99	114.89
1	A	466	UFT	N3-C2-N1	3.84	119.99	114.89
1	A	382	CFZ	C3'-C2'-C1'	3.84	107.78	103.13
1	A	43	UFT	C2'-C3'-C4'	3.84	107.37	102.40
1	B	268	CFZ	C2'-C3'-C4'	3.84	107.37	102.40
1	A	197	UFT	N3-C2-N1	3.84	119.99	114.89
1	A	695	UFT	N3-C2-N1	3.84	119.99	114.89
1	B	98	UFT	N3-C2-N1	3.84	119.99	114.89
1	B	322	UFT	N3-C2-N1	3.84	119.99	114.89
1	B	361	UFT	N3-C2-N1	3.84	119.99	114.89
1	B	389	UFT	N3-C2-N1	3.84	119.99	114.89
1	B	635	UFT	N3-C2-N1	3.84	119.99	114.89
1	B	114	CFZ	C3'-C2'-C1'	3.84	107.78	103.13
1	A	217	UFT	N3-C2-N1	3.84	119.99	114.89
1	B	8	UFT	N3-C2-N1	3.84	119.98	114.89
1	A	97	UFT	N3-C2-N1	3.84	119.98	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	UFT	N3-C2-N1	3.84	119.98	114.89
1	A	163	UFT	N3-C2-N1	3.84	119.98	114.89
1	B	338	CFZ	C2'-C3'-C4'	3.84	107.36	102.40
1	A	500	UFT	N3-C2-N1	3.84	119.98	114.89
1	A	502	UFT	N3-C2-N1	3.84	119.98	114.89
1	B	55	UFT	N3-C2-N1	3.84	119.98	114.89
1	A	192	UFT	N3-C2-N1	3.84	119.98	114.89
1	B	89	UFT	N3-C2-N1	3.83	119.98	114.89
1	A	62	UFT	N3-C2-N1	3.83	119.98	114.89
1	B	229	UFT	N3-C2-N1	3.83	119.98	114.89
1	B	430	UFT	N3-C2-N1	3.83	119.98	114.89
1	A	635	UFT	N3-C2-N1	3.83	119.98	114.89
1	B	687	UFT	N3-C2-N1	3.83	119.98	114.89
1	A	352	UFT	N3-C2-N1	3.83	119.98	114.89
1	A	602	UFT	N3-C2-N1	3.83	119.98	114.89
1	B	656	UFT	N3-C2-N1	3.83	119.98	114.89
1	B	663	UFT	N3-C2-N1	3.83	119.98	114.89
1	A	313	UFT	N3-C2-N1	3.83	119.98	114.89
1	B	439	CFZ	C3'-C2'-C1'	3.83	107.77	103.13
1	B	618	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	89	UFT	N3-C2-N1	3.83	119.97	114.89
1	B	106	UFT	N3-C2-N1	3.83	119.97	114.89
1	B	69	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	712	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	48	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	60	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	216	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	350	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	71	UFT	N3-C2-N1	3.83	119.97	114.89
1	B	153	UFT	N3-C2-N1	3.83	119.97	114.89
1	B	701	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	153	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	509	UFT	N3-C2-N1	3.83	119.97	114.89
1	B	607	UFT	N3-C2-N1	3.83	119.97	114.89
1	B	423	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	571	UFT	N3-C2-N1	3.83	119.97	114.89
1	A	358	UFT	N3-C2-N1	3.82	119.97	114.89
1	B	712	UFT	N3-C2-N1	3.82	119.97	114.89
1	A	389	UFT	N3-C2-N1	3.82	119.97	114.89
1	A	413	UFT	N3-C2-N1	3.82	119.97	114.89
1	B	555	UFT	N3-C2-N1	3.82	119.97	114.89
1	B	353	CFZ	C3'-C2'-C1'	3.82	107.76	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	618	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	202	UFT	C2'-C3'-C4'	3.82	107.34	102.40
1	B	469	CFZ	C3'-C2'-C1'	3.82	107.76	103.13
1	A	423	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	559	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	309	UFT	N3-C2-N1	3.82	119.96	114.89
1	B	493	UFT	C1'-N1-C2	3.82	124.49	117.57
1	A	50	UFT	N3-C2-N1	3.82	119.96	114.89
1	B	485	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	687	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	701	UFT	N3-C2-N1	3.82	119.96	114.89
1	B	141	UFT	N3-C2-N1	3.82	119.96	114.89
1	B	309	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	489	UFT	N3-C2-N1	3.82	119.96	114.89
1	B	260	UFT	N3-C2-N1	3.82	119.96	114.89
1	B	571	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	703	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	182	UFT	N3-C2-N1	3.82	119.96	114.89
1	B	192	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	233	UFT	N3-C2-N1	3.82	119.96	114.89
1	A	485	UFT	N3-C2-N1	3.82	119.96	114.89
1	B	519	UFT	N3-C2-N1	3.82	119.96	114.89
1	B	669	UFT	N3-C2-N1	3.82	119.96	114.89
1	B	80	UFT	N3-C2-N1	3.82	119.95	114.89
1	A	334	UFT	N3-C2-N1	3.82	119.95	114.89
1	B	398	UFT	N3-C2-N1	3.82	119.95	114.89
1	A	421	UFT	N3-C2-N1	3.81	119.95	114.89
1	A	33	UFT	N3-C2-N1	3.81	119.95	114.89
1	A	322	UFT	N3-C2-N1	3.81	119.95	114.89
1	B	621	UFT	N3-C2-N1	3.81	119.95	114.89
1	B	360	CFZ	C3'-C2'-C1'	3.81	107.75	103.13
1	A	365	UFT	N3-C2-N1	3.81	119.95	114.89
1	B	608	UFT	C3'-C2'-C1'	3.81	107.75	103.13
1	B	334	UFT	N3-C2-N1	3.81	119.95	114.89
1	A	549	UFT	N3-C2-N1	3.81	119.95	114.89
1	B	636	UFT	N3-C2-N1	3.81	119.95	114.89
1	A	260	UFT	N3-C2-N1	3.81	119.95	114.89
1	A	456	UFT	N3-C2-N1	3.81	119.95	114.89
1	A	610	CFZ	C3'-C2'-C1'	3.81	107.74	103.13
1	A	564	CFZ	C3'-C2'-C1'	3.81	107.74	103.13
1	B	74	UFT	N3-C2-N1	3.81	119.95	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	UFT	N3-C2-N1	3.81	119.95	114.89
1	B	233	UFT	N3-C2-N1	3.81	119.94	114.89
1	B	293	UFT	N3-C2-N1	3.81	119.94	114.89
1	A	175	UFT	N3-C2-N1	3.81	119.94	114.89
1	B	655	CFZ	C2'-C3'-C4'	3.81	107.32	102.40
1	B	175	UFT	N3-C2-N1	3.81	119.94	114.89
1	A	293	UFT	N3-C2-N1	3.81	119.94	114.89
1	A	608	UFT	N3-C2-N1	3.81	119.94	114.89
1	A	684	UFT	N3-C2-N1	3.81	119.94	114.89
1	A	143	UFT	C2'-C3'-C4'	3.81	107.32	102.40
1	B	265	UFT	N3-C2-N1	3.80	119.94	114.89
1	A	434	UFT	N3-C2-N1	3.80	119.94	114.89
1	B	581	UFT	N3-C2-N1	3.80	119.94	114.89
1	B	270	UFT	N3-C2-N1	3.80	119.94	114.89
1	B	549	UFT	N3-C2-N1	3.80	119.94	114.89
1	A	656	UFT	N3-C2-N1	3.80	119.94	114.89
1	A	196	UFT	N3-C2-N1	3.80	119.93	114.89
1	A	245	UFT	N3-C2-N1	3.80	119.93	114.89
1	A	80	UFT	N3-C2-N1	3.80	119.93	114.89
1	A	460	UFT	N3-C2-N1	3.80	119.93	114.89
1	A	534	UFT	N3-C2-N1	3.80	119.93	114.89
1	B	111	CFZ	C3'-C2'-C1'	3.80	107.73	103.13
1	B	544	UFT	C3'-C2'-C1'	3.80	107.73	103.13
1	B	216	UFT	N3-C2-N1	3.80	119.93	114.89
1	A	11	UFT	N3-C2-N1	3.79	119.93	114.89
1	A	229	UFT	N3-C2-N1	3.79	119.93	114.89
1	A	621	UFT	C2'-C3'-C4'	3.79	107.31	102.40
1	A	676	UFT	N3-C2-N1	3.79	119.92	114.89
1	B	352	UFT	N3-C2-N1	3.79	119.92	114.89
1	A	499	UFT	N3-C2-N1	3.79	119.92	114.89
1	B	8	UFT	C2'-C3'-C4'	3.79	107.30	102.40
1	A	338	CFZ	C2'-C3'-C4'	3.79	107.30	102.40
1	A	440	CFZ	C3'-C2'-C1'	3.79	107.72	103.13
1	A	469	CFZ	C3'-C2'-C1'	3.79	107.72	103.13
1	B	196	UFT	N3-C2-N1	3.79	119.92	114.89
1	A	111	CFZ	C3'-C2'-C1'	3.79	107.72	103.13
1	B	446	CFZ	C3'-C2'-C1'	3.79	107.72	103.13
1	A	377	UFT	N3-C2-N1	3.79	119.92	114.89
1	B	636	UFT	C3'-C2'-C1'	3.79	107.72	103.13
1	A	305	UFT	N3-C2-N1	3.79	119.92	114.89
1	B	402	UFT	N3-C2-N1	3.79	119.92	114.89
1	B	673	UFT	C3'-C2'-C1'	3.79	107.72	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	UFT	N3-C2-N1	3.79	119.92	114.89
1	A	402	UFT	N3-C2-N1	3.79	119.92	114.89
1	B	143	UFT	C2'-C3'-C4'	3.79	107.30	102.40
1	A	114	CFZ	C2'-C3'-C4'	3.79	107.29	102.40
1	B	353	CFZ	C2'-C3'-C4'	3.78	107.29	102.40
1	B	673	UFT	N3-C2-N1	3.78	119.91	114.89
1	B	676	UFT	N3-C2-N1	3.78	119.91	114.89
1	A	472	UFT	N3-C2-N1	3.78	119.91	114.89
1	A	202	UFT	C3'-C2'-C1'	3.78	107.71	103.13
1	B	460	UFT	N3-C2-N1	3.78	119.91	114.89
1	B	559	UFT	N3-C2-N1	3.78	119.91	114.89
1	B	590	UFT	C2'-C3'-C4'	3.78	107.29	102.40
1	B	59	UFT	N3-C2-N1	3.78	119.91	114.89
1	B	432	UFT	N3-C2-N1	3.78	119.91	114.89
1	A	581	UFT	N3-C2-N1	3.78	119.91	114.89
1	A	673	UFT	N3-C2-N1	3.78	119.91	114.89
1	A	114	CFZ	C3'-C2'-C1'	3.78	107.71	103.13
1	B	636	UFT	C2'-C3'-C4'	3.78	107.28	102.40
1	B	84	UFT	N3-C2-N1	3.78	119.90	114.89
1	A	92	UFT	N3-C2-N1	3.78	119.90	114.89
1	B	602	UFT	N3-C2-N1	3.78	119.90	114.89
1	B	384	CFZ	C3'-C2'-C1'	3.78	107.70	103.13
1	B	135	UFT	N3-C2-N1	3.78	119.90	114.89
1	A	544	UFT	C3'-C2'-C1'	3.78	107.70	103.13
1	A	583	CFZ	C2'-C3'-C4'	3.78	107.28	102.40
1	A	544	UFT	N3-C2-N1	3.78	119.90	114.89
1	A	204	UFT	N3-C2-N1	3.77	119.90	114.89
1	B	513	UFT	N3-C2-N1	3.77	119.90	114.89
1	B	13	UFT	C3'-C2'-C1'	3.77	107.70	103.13
1	A	98	UFT	N3-C2-N1	3.77	119.90	114.89
1	B	48	UFT	C2'-C3'-C4'	3.77	107.28	102.40
1	B	684	UFT	N3-C2-N1	3.77	119.89	114.89
1	B	703	UFT	N3-C2-N1	3.77	119.89	114.89
1	A	621	UFT	C3'-C2'-C1'	3.77	107.69	103.13
1	B	14	UFT	C2'-C1'-N1	-3.77	108.44	114.20
1	B	305	UFT	N3-C2-N1	3.77	119.89	114.89
1	B	282	CFZ	C3'-C2'-C1'	3.76	107.69	103.13
1	B	609	UFT	C3'-C2'-C1'	3.76	107.69	103.13
1	B	92	UFT	N3-C2-N1	3.76	119.89	114.89
1	A	492	CFZ	C3'-C2'-C1'	3.76	107.69	103.13
1	B	60	UFT	N3-C2-N1	3.76	119.89	114.89
1	B	464	UFT	N3-C2-N1	3.76	119.89	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	UFT	C3'-C2'-C1'	3.76	107.69	103.13
1	B	544	UFT	N3-C2-N1	3.76	119.88	114.89
1	A	669	UFT	N3-C2-N1	3.76	119.88	114.89
1	A	636	UFT	C2'-C3'-C4'	3.76	107.26	102.40
1	B	204	UFT	N3-C2-N1	3.76	119.88	114.89
1	B	621	UFT	C3'-C2'-C1'	3.76	107.68	103.13
1	B	472	UFT	N3-C2-N1	3.76	119.88	114.89
1	B	517	CFZ	C3'-C2'-C1'	3.76	107.68	103.13
1	B	377	UFT	N3-C2-N1	3.76	119.88	114.89
1	A	663	UFT	C2'-C3'-C4'	3.75	107.25	102.40
1	A	174	UFT	N3-C2-N1	3.75	119.87	114.89
1	B	174	UFT	N3-C2-N1	3.75	119.87	114.89
1	B	44	UFT	N3-C2-N1	3.75	119.87	114.89
1	A	530	UFT	N3-C2-N1	3.75	119.87	114.89
1	A	25	CFZ	C3'-C2'-C1'	3.75	107.67	103.13
1	A	116	UFT	C3'-C2'-C1'	3.75	107.67	103.13
1	B	555	UFT	C2'-C3'-C4'	3.75	107.25	102.40
1	B	663	UFT	C2'-C3'-C4'	3.75	107.25	102.40
1	A	555	UFT	C3'-C2'-C1'	3.75	107.67	103.13
1	B	43	UFT	N3-C2-N1	3.75	119.86	114.89
1	B	116	UFT	C3'-C2'-C1'	3.75	107.67	103.13
1	A	84	UFT	N3-C2-N1	3.74	119.86	114.89
1	A	44	UFT	N3-C2-N1	3.74	119.86	114.89
1	B	656	UFT	C3'-C2'-C1'	3.74	107.66	103.13
1	A	432	UFT	C2'-C1'-N1	-3.74	108.48	114.20
1	A	513	UFT	N3-C2-N1	3.74	119.85	114.89
1	A	182	UFT	C3'-C2'-C1'	3.74	107.66	103.13
1	A	105	UFT	N3-C2-N1	3.74	119.85	114.89
1	B	499	UFT	N3-C2-N1	3.74	119.85	114.89
1	B	15	CFZ	C2'-C3'-C4'	3.74	107.23	102.40
1	A	464	UFT	N3-C2-N1	3.74	119.85	114.89
1	B	621	UFT	C2'-C3'-C4'	3.73	107.23	102.40
1	A	42	UFT	N3-C2-N1	3.73	119.84	114.89
1	A	555	UFT	C2'-C3'-C4'	3.73	107.22	102.40
1	A	43	UFT	N3-C2-N1	3.73	119.83	114.89
1	A	62	UFT	C3'-C2'-C1'	3.72	107.64	103.13
1	A	302	UFT	N3-C2-N1	3.72	119.83	114.89
1	B	555	UFT	C3'-C2'-C1'	3.72	107.64	103.13
1	B	524	UFT	N3-C2-N1	3.72	119.83	114.89
1	B	74	UFT	C3'-C2'-C1'	3.72	107.63	103.13
1	A	362	CFZ	C2'-C3'-C4'	3.72	107.21	102.40
1	A	359	UFT	N3-C2-N1	3.71	119.82	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	UFT	C2'-C3'-C4'	3.71	107.20	102.40
1	B	607	UFT	C3'-C2'-C1'	3.71	107.63	103.13
1	B	302	UFT	N3-C2-N1	3.71	119.82	114.89
1	B	28	CFZ	O4'-C1'-N1	3.71	116.85	108.36
1	A	610	CFZ	C2'-C3'-C4'	3.71	107.20	102.40
1	A	282	CFZ	C3'-C2'-C1'	3.71	107.62	103.13
1	A	432	UFT	N3-C2-N1	3.71	119.81	114.89
1	B	606	UFT	C3'-C2'-C1'	3.71	107.62	103.13
1	B	182	UFT	C3'-C2'-C1'	3.70	107.61	103.13
1	B	564	CFZ	C3'-C2'-C1'	3.70	107.61	103.13
1	B	42	UFT	N3-C2-N1	3.70	119.80	114.89
1	A	323	CFZ	C3'-C2'-C1'	3.70	107.61	103.13
1	A	101	UFT	C2'-C3'-C4'	3.70	107.18	102.40
1	B	659	UFT	N3-C2-N1	3.69	119.79	114.89
1	A	659	UFT	N3-C2-N1	3.69	119.79	114.89
1	A	15	CFZ	C3'-C2'-C1'	3.69	107.60	103.13
1	B	481	UFT	N3-C2-N1	3.69	119.78	114.89
1	B	518	CFZ	C3'-C2'-C1'	3.69	107.59	103.13
1	B	174	UFT	C3'-C2'-C1'	3.68	107.59	103.13
1	B	544	UFT	C2'-C3'-C4'	3.68	107.16	102.40
1	B	535	UFT	N3-C2-N1	3.68	119.77	114.89
1	B	75	CFZ	C3'-C2'-C1'	3.68	107.58	103.13
1	B	105	UFT	N3-C2-N1	3.68	119.77	114.89
1	B	384	CFZ	C2'-C3'-C4'	3.68	107.15	102.40
1	B	75	CFZ	C2'-C3'-C4'	3.67	107.15	102.40
1	A	174	UFT	C3'-C2'-C1'	3.67	107.58	103.13
1	A	431	UFT	C3'-C2'-C1'	3.67	107.58	103.13
1	B	282	CFZ	C2'-C3'-C4'	3.67	107.14	102.40
1	A	215	UFT	C3'-C2'-C1'	3.67	107.57	103.13
1	A	28	CFZ	C2'-C1'-N1	-3.67	108.59	114.20
1	A	15	CFZ	C2'-C3'-C4'	3.67	107.14	102.40
1	A	631	CFZ	C3'-C2'-C1'	3.66	107.56	103.13
1	A	116	UFT	C2'-C3'-C4'	3.66	107.14	102.40
1	B	438	CFZ	C2'-C3'-C4'	3.66	107.13	102.40
1	A	535	UFT	N3-C2-N1	3.66	119.75	114.89
1	A	359	UFT	C3'-C2'-C1'	3.66	107.56	103.13
1	B	618	UFT	C3'-C2'-C1'	3.66	107.56	103.13
1	A	466	UFT	C3'-C2'-C1'	3.66	107.56	103.13
1	B	489	UFT	N3-C2-N1	3.66	119.74	114.89
1	A	62	UFT	C2'-C3'-C4'	3.65	107.12	102.40
1	B	631	CFZ	C3'-C2'-C1'	3.65	107.55	103.13
1	A	182	UFT	C2'-C3'-C4'	3.65	107.11	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	UFT	N3-C2-N1	3.65	119.73	114.89
1	B	679	CFZ	C3'-C2'-C1'	3.65	107.54	103.13
1	A	79	CFZ	C3'-C2'-C1'	3.64	107.54	103.13
1	B	347	UFT	C2'-C3'-C4'	3.63	107.10	102.40
1	B	321	CFZ	C3'-C2'-C1'	3.63	107.53	103.13
1	A	472	UFT	C3'-C2'-C1'	3.63	107.53	103.13
1	B	174	UFT	C2'-C3'-C4'	3.63	107.09	102.40
1	A	338	CFZ	C3'-C2'-C1'	3.63	107.52	103.13
1	B	111	CFZ	C2'-C3'-C4'	3.63	107.09	102.40
1	B	44	UFT	C5-C4-N3	3.63	120.26	114.84
1	B	74	UFT	C2'-C3'-C4'	3.62	107.09	102.40
1	A	361	UFT	C3'-C2'-C1'	3.62	107.52	103.13
1	B	182	UFT	C2'-C3'-C4'	3.62	107.08	102.40
1	B	270	UFT	C2'-C3'-C4'	3.62	107.08	102.40
1	B	466	UFT	C3'-C2'-C1'	3.62	107.51	103.13
1	A	89	UFT	C3'-C2'-C1'	3.61	107.51	103.13
1	B	79	CFZ	C3'-C2'-C1'	3.61	107.50	103.13
1	A	544	UFT	C2'-C3'-C4'	3.61	107.07	102.40
1	A	270	UFT	C2'-C3'-C4'	3.61	107.06	102.40
1	B	96	CFZ	C2'-C3'-C4'	3.60	107.06	102.40
1	A	444	CFZ	C2'-C3'-C4'	3.60	107.05	102.40
1	B	609	UFT	C2'-C3'-C4'	3.60	107.05	102.40
1	A	646	UFT	C3'-C2'-C1'	3.60	107.48	103.13
1	A	101	UFT	C3'-C2'-C1'	3.60	107.48	103.13
1	B	116	UFT	C2'-C3'-C4'	3.60	107.05	102.40
1	B	466	UFT	C2'-C3'-C4'	3.59	107.05	102.40
1	A	466	UFT	C2'-C3'-C4'	3.59	107.05	102.40
1	A	210	CFZ	C3'-C2'-C1'	3.59	107.48	103.13
1	A	618	UFT	C3'-C2'-C1'	3.59	107.48	103.13
1	B	518	CFZ	C2'-C3'-C4'	3.59	107.04	102.40
1	B	610	CFZ	C3'-C2'-C1'	3.59	107.48	103.13
1	A	135	UFT	C3'-C2'-C1'	3.59	107.47	103.13
1	B	556	CFZ	C2'-C3'-C4'	3.59	107.04	102.40
1	B	26	CFZ	C2'-C3'-C4'	3.58	107.03	102.40
1	B	60	UFT	C3'-C2'-C1'	3.58	107.47	103.13
1	A	631	CFZ	C2'-C3'-C4'	3.58	107.03	102.40
1	A	270	UFT	C3'-C2'-C1'	3.58	107.46	103.13
1	A	350	UFT	C5-C4-N3	3.58	120.19	114.84
1	A	438	CFZ	C2'-C3'-C4'	3.57	107.02	102.40
1	A	656	UFT	C3'-C2'-C1'	3.57	107.46	103.13
1	A	200	UFT	C3'-C2'-C1'	3.57	107.45	103.13
1	B	89	UFT	C3'-C2'-C1'	3.57	107.45	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	CFZ	C3'-C2'-C1'	3.57	107.45	103.13
1	A	111	CFZ	C2'-C3'-C4'	3.57	107.01	102.40
1	B	618	UFT	C2'-C3'-C4'	3.57	107.01	102.40
1	A	69	UFT	C3'-C2'-C1'	3.57	107.45	103.13
1	B	270	UFT	C3'-C2'-C1'	3.57	107.45	103.13
1	B	126	UFT	C3'-C2'-C1'	3.57	107.45	103.13
1	B	15	CFZ	C3'-C2'-C1'	3.56	107.45	103.13
1	B	59	UFT	C2'-C3'-C4'	3.56	107.01	102.40
1	A	301	UFT	C2'-C3'-C4'	3.56	107.01	102.40
1	A	503	UFT	C3'-C2'-C1'	3.56	107.44	103.13
1	B	360	CFZ	C2'-C3'-C4'	3.56	107.01	102.40
1	A	381	CFZ	C3'-C2'-C1'	3.56	107.44	103.13
1	B	469	CFZ	C2'-C3'-C4'	3.56	107.00	102.40
1	B	62	UFT	C3'-C2'-C1'	3.56	107.44	103.13
1	A	126	UFT	C3'-C2'-C1'	3.56	107.44	103.13
1	A	609	UFT	C3'-C2'-C1'	3.55	107.43	103.13
1	B	210	CFZ	C2'-C3'-C4'	3.55	106.99	102.40
1	A	140	CFZ	C3'-C2'-C1'	3.55	107.43	103.13
1	A	234	CFZ	C3'-C2'-C1'	3.55	107.43	103.13
1	B	335	CFZ	C3'-C2'-C1'	3.55	107.43	103.13
1	B	646	UFT	C3'-C2'-C1'	3.55	107.42	103.13
1	B	89	UFT	C2'-C3'-C4'	3.54	106.98	102.40
1	B	210	CFZ	C3'-C2'-C1'	3.54	107.42	103.13
1	A	469	CFZ	C2'-C3'-C4'	3.54	106.98	102.40
1	A	344	UFT	C2'-C3'-C4'	3.54	106.97	102.40
1	A	74	UFT	C3'-C2'-C1'	3.54	107.41	103.13
1	A	489	UFT	C2'-C3'-C4'	3.53	106.97	102.40
1	B	200	UFT	C2'-C3'-C4'	3.53	106.97	102.40
1	B	334	UFT	C2'-C3'-C4'	3.53	106.97	102.40
1	A	472	UFT	C2'-C3'-C4'	3.53	106.97	102.40
1	B	200	UFT	C3'-C2'-C1'	3.53	107.41	103.13
1	A	25	CFZ	C2'-C3'-C4'	3.53	106.96	102.40
1	A	352	UFT	C3'-C2'-C1'	3.53	107.40	103.13
1	B	631	CFZ	C2'-C3'-C4'	3.53	106.96	102.40
1	B	471	UFT	C2'-C1'-N1	-3.53	108.81	114.20
1	B	473	CFZ	C3'-C2'-C1'	3.52	107.40	103.13
1	A	154	UFT	C2'-C3'-C4'	3.52	106.95	102.40
1	B	301	UFT	C2'-C3'-C4'	3.52	106.95	102.40
1	A	382	CFZ	C2'-C3'-C4'	3.52	106.95	102.40
1	A	69	UFT	C2'-C3'-C4'	3.52	106.95	102.40
1	B	576	CFZ	C2'-C3'-C4'	3.52	106.95	102.40
1	B	141	UFT	C3'-C2'-C1'	3.51	107.39	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	CFZ	C3'-C2'-C1'	3.51	107.39	103.13
1	A	210	CFZ	C2'-C3'-C4'	3.51	106.94	102.40
1	B	486	CFZ	C3'-C2'-C1'	3.51	107.38	103.13
1	B	556	CFZ	C3'-C2'-C1'	3.51	107.38	103.13
1	A	141	UFT	C3'-C2'-C1'	3.51	107.38	103.13
1	B	302	UFT	C5-C4-N3	3.50	120.08	114.84
1	A	302	UFT	C5-C4-N3	3.50	120.08	114.84
1	A	618	UFT	C2'-C3'-C4'	3.49	106.92	102.40
1	B	456	UFT	C2'-C1'-N1	-3.49	108.86	114.20
1	A	305	UFT	C5-C4-N3	3.49	120.07	114.84
1	B	361	UFT	C5-C4-N3	3.49	120.07	114.84
1	A	44	UFT	C5-C4-N3	3.49	120.06	114.84
1	A	89	UFT	C2'-C3'-C4'	3.49	106.91	102.40
1	A	459	CFZ	C3'-C2'-C1'	3.49	107.36	103.13
1	A	335	CFZ	C3'-C2'-C1'	3.49	107.35	103.13
1	A	500	UFT	C3'-C2'-C1'	3.49	107.35	103.13
1	B	315	CFZ	C3'-C2'-C1'	3.49	107.35	103.13
1	A	94	UFT	C2'-C3'-C4'	3.48	106.90	102.40
1	A	334	UFT	C2'-C3'-C4'	3.48	106.90	102.40
1	A	398	UFT	C5-C4-N3	3.48	120.05	114.84
1	A	471	UFT	C5-C4-N3	3.48	120.05	114.84
1	B	305	UFT	C2'-C3'-C4'	3.48	106.90	102.40
1	A	628	UFT	C2'-C3'-C4'	3.48	106.90	102.40
1	B	140	CFZ	C3'-C2'-C1'	3.47	107.34	103.13
1	A	142	UFT	C5-C4-N3	3.47	120.03	114.84
1	B	169	UFT	C3'-C2'-C1'	3.47	107.33	103.13
1	A	48	UFT	C3'-C2'-C1'	3.47	107.33	103.13
1	B	500	UFT	C3'-C2'-C1'	3.47	107.33	103.13
1	B	377	UFT	C3'-C2'-C1'	3.47	107.33	103.13
1	A	456	UFT	C2'-C1'-N1	-3.46	108.90	114.20
1	B	74	UFT	C5-C4-N3	3.46	120.02	114.84
1	A	701	UFT	C3'-C2'-C1'	3.46	107.32	103.13
1	B	313	UFT	C5-C4-N3	3.46	120.02	114.84
1	A	366	UFT	C3'-C2'-C1'	3.46	107.32	103.13
1	B	431	UFT	C3'-C2'-C1'	3.46	107.32	103.13
1	A	174	UFT	C2'-C3'-C4'	3.46	106.87	102.40
1	B	608	UFT	C5-C4-N3	3.46	120.02	114.84
1	A	621	UFT	C5-C4-N3	3.46	120.01	114.84
1	B	366	UFT	C3'-C2'-C1'	3.46	107.32	103.13
1	A	74	UFT	C5-C4-N3	3.46	120.01	114.84
1	B	398	UFT	C5-C4-N3	3.46	120.01	114.84
1	B	662	UFT	C5-C4-N3	3.45	120.01	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	CFZ	C2'-C3'-C4'	3.45	106.87	102.40
1	B	98	UFT	C5-C4-N3	3.45	120.00	114.84
1	A	336	UFT	C5-C4-N3	3.45	120.00	114.84
1	A	636	UFT	C5-C4-N3	3.45	120.00	114.84
1	B	34	CFZ	C3'-C2'-C1'	3.45	107.31	103.13
1	A	61	UFT	C5-C4-N3	3.45	120.00	114.84
1	A	564	CFZ	C2'-C3'-C4'	3.45	106.86	102.40
1	A	197	UFT	C5-C4-N3	3.45	120.00	114.84
1	A	169	UFT	C3'-C2'-C1'	3.45	107.31	103.13
1	A	13	UFT	C3'-C2'-C1'	3.45	107.31	103.13
1	B	459	CFZ	C2'-C3'-C4'	3.45	106.86	102.40
1	B	430	UFT	C5-C4-N3	3.45	120.00	114.84
1	A	493	UFT	C3'-C2'-C1'	3.45	107.30	103.13
1	A	74	UFT	C2'-C3'-C4'	3.45	106.86	102.40
1	B	434	UFT	C5-C4-N3	3.45	120.00	114.84
1	A	493	UFT	C5-C4-N3	3.45	120.00	114.84
1	B	182	UFT	C5-C4-N3	3.44	119.99	114.84
1	B	305	UFT	C5-C4-N3	3.44	119.99	114.84
1	A	62	UFT	C5-C4-N3	3.44	119.99	114.84
1	B	154	UFT	C2'-C3'-C4'	3.44	106.85	102.40
1	B	502	UFT	C3'-C2'-C1'	3.44	107.30	103.13
1	B	62	UFT	C5-C4-N3	3.44	119.99	114.84
1	A	143	UFT	C5-C4-N3	3.44	119.99	114.84
1	B	89	UFT	C5-C4-N3	3.44	119.99	114.84
1	B	519	UFT	C5-C4-N3	3.44	119.99	114.84
1	A	663	UFT	C5-C4-N3	3.44	119.99	114.84
1	A	471	UFT	C2'-C1'-N1	-3.44	108.94	114.20
1	B	61	UFT	C5-C4-N3	3.44	119.99	114.84
1	B	432	UFT	C5-C4-N3	3.44	119.99	114.84
1	A	60	UFT	C5-C4-N3	3.44	119.99	114.84
1	A	89	UFT	C5-C4-N3	3.44	119.99	114.84
1	B	143	UFT	C5-C4-N3	3.44	119.99	114.84
1	B	471	UFT	C5-C4-N3	3.44	119.99	114.84
1	B	69	UFT	C3'-C2'-C1'	3.44	107.30	103.13
1	B	88	UFT	C5-C4-N3	3.44	119.99	114.84
1	A	101	UFT	C5-C4-N3	3.44	119.99	114.84
1	A	170	UFT	C5-C4-N3	3.44	119.99	114.84
1	B	170	UFT	C5-C4-N3	3.44	119.99	114.84
1	B	126	UFT	C5-C4-N3	3.44	119.98	114.84
1	A	305	UFT	C2'-C3'-C4'	3.44	106.85	102.40
1	A	377	UFT	C3'-C2'-C1'	3.44	107.29	103.13
1	B	456	UFT	C5-C4-N3	3.44	119.98	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	UFT	C5-C4-N3	3.43	119.98	114.84
1	A	571	UFT	C5-C4-N3	3.43	119.98	114.84
1	B	197	UFT	C5-C4-N3	3.43	119.98	114.84
1	B	352	UFT	C5-C4-N3	3.43	119.98	114.84
1	A	635	UFT	C5-C4-N3	3.43	119.98	114.84
1	A	315	CFZ	C3'-C2'-C1'	3.43	107.29	103.13
1	A	126	UFT	C5-C4-N3	3.43	119.98	114.84
1	A	403	UFT	C5-C4-N3	3.43	119.98	114.84
1	B	609	UFT	C5-C4-N3	3.43	119.98	114.84
1	B	621	UFT	C5-C4-N3	3.43	119.98	114.84
1	B	169	UFT	C5-C4-N3	3.43	119.98	114.84
1	B	555	UFT	C5-C4-N3	3.43	119.98	114.84
1	A	554	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	265	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	524	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	635	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	103	CFZ	C3'-C2'-C1'	3.43	107.28	103.13
1	A	160	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	696	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	459	CFZ	C2'-C3'-C4'	3.43	106.83	102.40
1	A	456	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	359	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	485	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	554	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	559	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	571	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	160	UFT	C3'-C2'-C1'	3.43	107.28	103.13
1	A	154	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	160	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	182	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	245	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	608	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	582	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	582	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	609	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	155	UFT	C5-C4-N3	3.43	119.97	114.84
1	A	347	UFT	C5-C4-N3	3.43	119.97	114.84
1	B	94	UFT	C5-C4-N3	3.42	119.96	114.84
1	A	169	UFT	C5-C4-N3	3.42	119.96	114.84
1	B	403	UFT	C5-C4-N3	3.42	119.96	114.84
1	B	663	UFT	C5-C4-N3	3.42	119.96	114.84
1	B	69	UFT	C5-C4-N3	3.42	119.96	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	UFT	C5-C4-N3	3.42	119.96	114.84
1	B	618	UFT	C5-C4-N3	3.42	119.96	114.84
1	B	190	UFT	C5-C4-N3	3.42	119.96	114.84
1	A	270	UFT	C5-C4-N3	3.42	119.96	114.84
1	B	423	UFT	C5-C4-N3	3.42	119.96	114.84
1	A	666	UFT	C5-C4-N3	3.42	119.96	114.84
1	B	202	UFT	C5-C4-N3	3.42	119.96	114.84
1	B	653	UFT	C5-C4-N3	3.42	119.96	114.84
1	B	135	UFT	C3'-C2'-C1'	3.42	107.27	103.13
1	A	296	UFT	C5-C4-N3	3.42	119.96	114.84
1	A	545	UFT	C5-C4-N3	3.42	119.96	114.84
1	A	608	UFT	C3'-C2'-C1'	3.42	107.27	103.13
1	B	101	UFT	C5-C4-N3	3.42	119.96	114.84
1	A	71	UFT	C3'-C2'-C1'	3.42	107.27	103.13
1	B	322	UFT	C5-C4-N3	3.42	119.96	114.84
1	A	708	UFT	C5-C4-N3	3.42	119.96	114.84
1	A	447	UFT	C5-C4-N3	3.42	119.95	114.84
1	A	500	UFT	C5-C4-N3	3.42	119.95	114.84
1	B	504	UFT	C5-C4-N3	3.42	119.95	114.84
1	A	620	CFZ	C3'-C2'-C1'	3.42	107.27	103.13
1	B	689	UFT	C5-C4-N3	3.42	119.95	114.84
1	A	690	UFT	C5-C4-N3	3.42	119.95	114.84
1	A	50	UFT	C5-C4-N3	3.42	119.95	114.84
1	B	336	UFT	C5-C4-N3	3.42	119.95	114.84
1	A	581	UFT	C5-C4-N3	3.42	119.95	114.84
1	A	489	UFT	C5-C4-N3	3.42	119.95	114.84
1	A	618	UFT	C5-C4-N3	3.42	119.95	114.84
1	A	423	UFT	C5-C4-N3	3.42	119.95	114.84
1	B	593	UFT	C5-C4-N3	3.42	119.95	114.84
1	A	695	UFT	C5-C4-N3	3.42	119.95	114.84
1	A	137	UFT	C5-C4-N3	3.42	119.95	114.84
1	B	545	UFT	C5-C4-N3	3.42	119.95	114.84
1	B	673	UFT	C5-C4-N3	3.42	119.95	114.84
1	B	437	UFT	C2'-C3'-C4'	3.42	106.82	102.40
1	A	434	UFT	C5-C4-N3	3.41	119.95	114.84
1	A	720	UFT	C5-C4-N3	3.41	119.95	114.84
1	A	234	CFZ	C2'-C3'-C4'	3.41	106.81	102.40
1	B	86	UFT	C5-C4-N3	3.41	119.95	114.84
1	B	296	UFT	C5-C4-N3	3.41	119.95	114.84
1	A	432	UFT	C5-C4-N3	3.41	119.95	114.84
1	A	593	UFT	C5-C4-N3	3.41	119.95	114.84
1	A	719	UFT	C5-C4-N3	3.41	119.95	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	UFT	C5-C4-N3	3.41	119.95	114.84
1	B	542	UFT	C5-C4-N3	3.41	119.95	114.84
1	A	676	UFT	C3'-C2'-C1'	3.41	107.26	103.13
1	A	116	UFT	C5-C4-N3	3.41	119.95	114.84
1	A	190	UFT	C5-C4-N3	3.41	119.95	114.84
1	B	301	UFT	C5-C4-N3	3.41	119.95	114.84
1	B	84	UFT	C5-C4-N3	3.41	119.94	114.84
1	B	270	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	472	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	55	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	97	UFT	C5-C4-N3	3.41	119.94	114.84
1	B	115	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	84	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	204	UFT	C5-C4-N3	3.41	119.94	114.84
1	B	215	UFT	C5-C4-N3	3.41	119.94	114.84
1	B	466	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	662	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	625	CFZ	C3'-C2'-C1'	3.41	107.26	103.13
1	B	71	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	430	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	577	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	301	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	402	UFT	C5-C4-N3	3.41	119.94	114.84
1	B	141	UFT	C5-C4-N3	3.41	119.94	114.84
1	B	174	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	229	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	260	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	696	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	86	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	265	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	689	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	190	UFT	C3'-C2'-C1'	3.41	107.26	103.13
1	A	535	UFT	C2'-C1'-N1	-3.41	108.99	114.20
1	B	154	UFT	C5-C4-N3	3.41	119.94	114.84
1	B	309	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	466	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	555	UFT	C5-C4-N3	3.41	119.94	114.84
1	B	204	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	334	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	542	UFT	C5-C4-N3	3.41	119.94	114.84
1	B	719	UFT	C5-C4-N3	3.41	119.94	114.84
1	A	98	UFT	C5-C4-N3	3.41	119.94	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	UFT	C5-C4-N3	3.41	119.94	114.84
1	B	260	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	344	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	365	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	500	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	606	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	701	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	712	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	266	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	116	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	366	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	636	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	19	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	684	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	701	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	266	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	365	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	115	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	142	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	229	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	653	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	202	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	309	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	564	CFZ	C2'-C3'-C4'	3.40	106.80	102.40
1	A	437	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	559	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	687	UFT	C5-C4-N3	3.40	119.93	114.84
1	B	153	UFT	C5-C4-N3	3.40	119.93	114.84
1	A	283	UFT	C5-C4-N3	3.40	119.92	114.84
1	B	334	UFT	C5-C4-N3	3.40	119.92	114.84
1	B	581	UFT	C5-C4-N3	3.40	119.92	114.84
1	B	606	UFT	C5-C4-N3	3.40	119.92	114.84
1	A	360	CFZ	C3'-C2'-C1'	3.40	107.25	103.13
1	B	402	UFT	C5-C4-N3	3.40	119.92	114.84
1	A	106	UFT	C5-C4-N3	3.40	119.92	114.84
1	B	217	UFT	C5-C4-N3	3.40	119.92	114.84
1	A	293	UFT	C5-C4-N3	3.40	119.92	114.84
1	B	347	UFT	C5-C4-N3	3.40	119.92	114.84
1	B	366	UFT	C5-C4-N3	3.40	119.92	114.84
1	B	549	UFT	C5-C4-N3	3.40	119.92	114.84
1	B	695	UFT	C5-C4-N3	3.40	119.92	114.84
1	A	14	UFT	C5-C4-N3	3.39	119.92	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	UFT	C5-C4-N3	3.39	119.92	114.84
1	A	88	UFT	C5-C4-N3	3.39	119.92	114.84
1	A	174	UFT	C5-C4-N3	3.39	119.92	114.84
1	A	590	UFT	C5-C4-N3	3.39	119.92	114.84
1	B	534	UFT	C5-C4-N3	3.39	119.92	114.84
1	A	13	UFT	C5-C4-N3	3.39	119.92	114.84
1	A	437	UFT	C2'-C3'-C4'	3.39	106.79	102.40
1	A	502	UFT	C3'-C2'-C1'	3.39	107.24	103.13
1	A	606	UFT	C3'-C2'-C1'	3.39	107.24	103.13
1	B	11	UFT	C5-C4-N3	3.39	119.92	114.84
1	B	14	UFT	C5-C4-N3	3.39	119.92	114.84
1	A	141	UFT	C5-C4-N3	3.39	119.92	114.84
1	A	208	UFT	C5-C4-N3	3.39	119.92	114.84
1	B	530	UFT	C5-C4-N3	3.39	119.92	114.84
1	B	666	UFT	C5-C4-N3	3.39	119.92	114.84
1	B	55	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	97	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	283	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	8	UFT	C5-C4-N3	3.39	119.91	114.84
1	A	431	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	701	UFT	C3'-C2'-C1'	3.39	107.23	103.13
1	B	112	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	509	UFT	C5-C4-N3	3.39	119.91	114.84
1	A	8	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	214	UFT	C5-C4-N3	3.39	119.91	114.84
1	A	154	UFT	C3'-C2'-C1'	3.39	107.23	103.13
1	A	509	UFT	C5-C4-N3	3.39	119.91	114.84
1	A	633	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	208	UFT	C5-C4-N3	3.39	119.91	114.84
1	A	534	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	607	UFT	C5-C4-N3	3.39	119.91	114.84
1	A	646	UFT	C5-C4-N3	3.39	119.91	114.84
1	A	607	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	708	UFT	C5-C4-N3	3.39	119.91	114.84
1	A	559	UFT	C3'-C2'-C1'	3.39	107.23	103.13
1	A	94	UFT	C5-C4-N3	3.39	119.91	114.84
1	A	192	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	329	UFT	C5-C4-N3	3.39	119.91	114.84
1	B	535	UFT	C2'-C1'-N1	-3.39	109.03	114.20
1	A	620	CFZ	C2'-C3'-C4'	3.39	106.78	102.40
1	A	519	UFT	C5-C4-N3	3.39	119.91	114.84
1	A	503	UFT	C2'-C3'-C4'	3.38	106.78	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	431	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	154	UFT	C3'-C2'-C1'	3.38	107.23	103.13
1	B	48	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	50	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	80	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	175	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	633	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	712	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	232	CFZ	C3'-C2'-C1'	3.38	107.23	103.13
1	A	59	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	690	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	628	UFT	C2'-C3'-C4'	3.38	106.77	102.40
1	A	175	UFT	C5-C4-N3	3.38	119.90	114.84
1	A	359	UFT	C1'-N1-C2	3.38	123.69	117.57
1	B	59	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	106	UFT	C5-C4-N3	3.38	119.90	114.84
1	A	94	UFT	C3'-C2'-C1'	3.38	107.22	103.13
1	B	293	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	523	CFZ	C3'-C2'-C1'	3.38	107.22	103.13
1	A	500	UFT	C2'-C3'-C4'	3.38	106.77	102.40
1	A	19	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	33	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	577	UFT	C5-C4-N3	3.38	119.90	114.84
1	B	108	UFT	C5-C4-N3	3.38	119.89	114.84
1	B	137	UFT	C5-C4-N3	3.38	119.89	114.84
1	B	447	UFT	C5-C4-N3	3.38	119.89	114.84
1	B	251	UFT	C5-C4-N3	3.38	119.89	114.84
1	A	499	UFT	C5-C4-N3	3.38	119.89	114.84
1	B	506	CFZ	C2'-C3'-C4'	3.38	106.77	102.40
1	A	383	CFZ	C3'-C2'-C1'	3.38	107.22	103.13
1	B	13	UFT	C5-C4-N3	3.38	119.89	114.84
1	A	163	UFT	C5-C4-N3	3.38	119.89	114.84
1	B	590	UFT	C5-C4-N3	3.38	119.89	114.84
1	A	260	UFT	C2'-C1'-N1	-3.38	109.04	114.20
1	B	687	UFT	C5-C4-N3	3.37	119.89	114.84
1	A	384	CFZ	C3'-C2'-C1'	3.37	107.22	103.13
1	B	620	CFZ	C3'-C2'-C1'	3.37	107.22	103.13
1	A	48	UFT	C5-C4-N3	3.37	119.89	114.84
1	A	464	UFT	C5-C4-N3	3.37	119.89	114.84
1	A	544	UFT	C5-C4-N3	3.37	119.89	114.84
1	A	602	UFT	C5-C4-N3	3.37	119.89	114.84
1	B	502	UFT	C5-C4-N3	3.37	119.89	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	UFT	C5-C4-N3	3.37	119.89	114.84
1	A	549	UFT	C5-C4-N3	3.37	119.89	114.84
1	B	354	CFZ	C3'-C2'-C1'	3.37	107.21	103.13
1	B	92	UFT	C5-C4-N3	3.37	119.89	114.84
1	A	431	UFT	C2'-C3'-C4'	3.37	106.76	102.40
1	B	200	UFT	C5-C4-N3	3.37	119.88	114.84
1	A	329	UFT	C5-C4-N3	3.37	119.88	114.84
1	A	460	UFT	C5-C4-N3	3.37	119.88	114.84
1	A	628	UFT	C5-C4-N3	3.37	119.88	114.84
1	B	43	UFT	C1'-N1-C2	3.37	123.67	117.57
1	A	609	UFT	C2'-C3'-C4'	3.37	106.76	102.40
1	B	610	CFZ	C2'-C3'-C4'	3.37	106.76	102.40
1	B	334	UFT	C3'-C2'-C1'	3.37	107.21	103.13
1	A	200	UFT	C5-C4-N3	3.37	119.88	114.84
1	A	389	UFT	C5-C4-N3	3.37	119.88	114.84
1	A	498	CFZ	C3'-C2'-C1'	3.37	107.21	103.13
1	B	602	UFT	C5-C4-N3	3.37	119.88	114.84
1	B	703	UFT	C5-C4-N3	3.37	119.88	114.84
1	A	153	UFT	C5-C4-N3	3.37	119.88	114.84
1	B	437	UFT	C5-C4-N3	3.37	119.88	114.84
1	A	60	UFT	C3'-C2'-C1'	3.37	107.21	103.13
1	B	202	UFT	C3'-C2'-C1'	3.37	107.21	103.13
1	B	389	UFT	C5-C4-N3	3.37	119.88	114.84
1	A	71	UFT	C2'-C3'-C4'	3.37	106.75	102.40
1	A	344	UFT	C5-C4-N3	3.37	119.88	114.84
1	A	377	UFT	C2'-C3'-C4'	3.37	106.75	102.40
1	B	163	UFT	C5-C4-N3	3.37	119.88	114.84
1	B	212	CFZ	C3'-C2'-C1'	3.37	107.20	103.13
1	B	464	UFT	C5-C4-N3	3.36	119.87	114.84
1	A	530	UFT	C5-C4-N3	3.36	119.87	114.84
1	A	11	UFT	C5-C4-N3	3.36	119.87	114.84
1	B	60	UFT	C5-C4-N3	3.36	119.87	114.84
1	A	71	UFT	C5-C4-N3	3.36	119.87	114.84
1	B	499	UFT	C5-C4-N3	3.36	119.87	114.84
1	B	628	UFT	C5-C4-N3	3.36	119.87	114.84
1	A	92	UFT	C5-C4-N3	3.36	119.87	114.84
1	A	703	UFT	C5-C4-N3	3.36	119.87	114.84
1	A	108	UFT	C5-C4-N3	3.36	119.87	114.84
1	B	367	UFT	C5-C4-N3	3.36	119.87	114.84
1	A	112	UFT	C5-C4-N3	3.36	119.87	114.84
1	B	684	UFT	C5-C4-N3	3.36	119.87	114.84
1	B	500	UFT	C2'-C3'-C4'	3.36	106.74	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	UFT	C5-C4-N3	3.36	119.87	114.84
1	A	42	UFT	C5-C4-N3	3.36	119.86	114.84
1	B	233	UFT	C5-C4-N3	3.36	119.86	114.84
1	B	472	UFT	C5-C4-N3	3.36	119.86	114.84
1	A	251	UFT	C5-C4-N3	3.36	119.86	114.84
1	A	421	UFT	C5-C4-N3	3.36	119.86	114.84
1	B	481	UFT	C5-C4-N3	3.36	119.86	114.84
1	A	502	UFT	C5-C4-N3	3.36	119.86	114.84
1	B	190	UFT	C3'-C2'-C1'	3.36	107.19	103.13
1	B	625	CFZ	C3'-C2'-C1'	3.36	107.19	103.13
1	A	503	UFT	C5-C4-N3	3.36	119.86	114.84
1	B	628	UFT	C3'-C2'-C1'	3.36	107.19	103.13
1	A	233	UFT	C5-C4-N3	3.36	119.86	114.84
1	A	218	CFZ	C2'-C3'-C4'	3.36	106.74	102.40
1	B	498	CFZ	C3'-C2'-C1'	3.36	107.19	103.13
1	A	126	UFT	C2'-C3'-C4'	3.35	106.74	102.40
1	A	196	UFT	C5-C4-N3	3.35	119.86	114.84
1	B	196	UFT	C5-C4-N3	3.35	119.86	114.84
1	B	669	UFT	C5-C4-N3	3.35	119.86	114.84
1	A	367	UFT	C5-C4-N3	3.35	119.86	114.84
1	B	544	UFT	C5-C4-N3	3.35	119.86	114.84
1	A	492	CFZ	C2'-C3'-C4'	3.35	106.73	102.40
1	B	179	UFT	C5-C4-N3	3.35	119.85	114.84
1	B	517	CFZ	C2'-C3'-C4'	3.35	106.73	102.40
1	A	481	UFT	C5-C4-N3	3.35	119.85	114.84
1	B	434	UFT	C3'-C2'-C1'	3.35	107.19	103.13
1	A	179	UFT	C5-C4-N3	3.35	119.85	114.84
1	B	377	UFT	C5-C4-N3	3.35	119.85	114.84
1	A	513	UFT	C5-C4-N3	3.35	119.85	114.84
1	A	377	UFT	C5-C4-N3	3.35	119.85	114.84
1	A	673	UFT	C5-C4-N3	3.35	119.84	114.84
1	B	485	UFT	C5-C4-N3	3.34	119.84	114.84
1	B	513	UFT	C5-C4-N3	3.34	119.84	114.84
1	A	576	CFZ	C2'-C3'-C4'	3.34	106.72	102.40
1	A	506	CFZ	C2'-C3'-C4'	3.34	106.72	102.40
1	B	421	UFT	C5-C4-N3	3.34	119.84	114.84
1	B	656	UFT	C5-C4-N3	3.34	119.84	114.84
1	A	628	UFT	C3'-C2'-C1'	3.34	107.17	103.13
1	B	646	UFT	C5-C4-N3	3.34	119.83	114.84
1	A	332	CFZ	C2'-C3'-C4'	3.34	106.72	102.40
1	B	335	CFZ	C2'-C3'-C4'	3.34	106.71	102.40
1	A	361	UFT	C5-C4-N3	3.34	119.83	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	UFT	C5-C4-N3	3.33	119.83	114.84
1	B	460	UFT	C5-C4-N3	3.33	119.83	114.84
1	B	676	UFT	C5-C4-N3	3.33	119.83	114.84
1	A	61	UFT	C3'-C2'-C1'	3.33	107.17	103.13
1	B	676	UFT	C3'-C2'-C1'	3.33	107.17	103.13
1	A	413	UFT	C5-C4-N3	3.33	119.83	114.84
1	B	377	UFT	C2'-C3'-C4'	3.33	106.71	102.40
1	A	629	UFT	C5-C4-N3	3.33	119.83	114.84
1	A	669	UFT	C5-C4-N3	3.33	119.83	114.84
1	A	656	UFT	C5-C4-N3	3.33	119.82	114.84
1	B	160	UFT	C3'-C2'-C1'	3.33	107.16	103.13
1	A	632	CFZ	C3'-C2'-C1'	3.33	107.16	103.13
1	B	629	UFT	C5-C4-N3	3.33	119.82	114.84
1	B	489	UFT	C5-C4-N3	3.33	119.82	114.84
1	B	260	UFT	C2'-C1'-N1	-3.33	109.12	114.20
1	B	62	UFT	C2'-C3'-C4'	3.33	106.70	102.40
1	A	33	UFT	C5-C4-N3	3.32	119.81	114.84
1	B	332	CFZ	C2'-C3'-C4'	3.32	106.69	102.40
1	A	369	CFZ	C3'-C2'-C1'	3.32	107.15	103.13
1	A	403	UFT	C3'-C2'-C1'	3.32	107.15	103.13
1	B	354	CFZ	C2'-C3'-C4'	3.32	106.69	102.40
1	B	216	UFT	C3'-C2'-C1'	3.32	107.14	103.13
1	A	105	UFT	C5-C4-N3	3.31	119.80	114.84
1	A	135	UFT	C5-C4-N3	3.31	119.80	114.84
1	B	576	CFZ	C3'-C2'-C1'	3.31	107.14	103.13
1	A	80	UFT	C5-C4-N3	3.31	119.80	114.84
1	A	344	UFT	C3'-C2'-C1'	3.31	107.14	103.13
1	B	632	CFZ	C3'-C2'-C1'	3.31	107.14	103.13
1	A	473	CFZ	C3'-C2'-C1'	3.31	107.14	103.13
1	B	126	UFT	C2'-C3'-C4'	3.31	106.68	102.40
1	A	676	UFT	C5-C4-N3	3.31	119.79	114.84
1	B	218	CFZ	C3'-C2'-C1'	3.31	107.14	103.13
1	A	590	UFT	C3'-C2'-C1'	3.31	107.13	103.13
1	B	105	UFT	C5-C4-N3	3.30	119.78	114.84
1	A	190	UFT	C2'-C3'-C4'	3.30	106.67	102.40
1	B	659	UFT	C5-C4-N3	3.30	119.77	114.84
1	A	434	UFT	C3'-C2'-C1'	3.30	107.12	103.13
1	A	372	CFZ	C3'-C2'-C1'	3.30	107.12	103.13
1	B	61	UFT	C3'-C2'-C1'	3.30	107.12	103.13
1	A	43	UFT	C1'-N1-C2	3.30	123.54	117.57
1	B	464	UFT	C3'-C2'-C1'	3.29	107.12	103.13
1	B	69	UFT	C2'-C3'-C4'	3.29	106.66	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	UFT	C5-C4-N3	3.29	119.77	114.84
1	B	535	UFT	C5-C4-N3	3.29	119.77	114.84
1	A	60	UFT	C2'-C3'-C4'	3.29	106.66	102.40
1	A	493	UFT	C2'-C3'-C4'	3.29	106.66	102.40
1	B	48	UFT	C3'-C2'-C1'	3.29	107.12	103.13
1	A	535	UFT	C5-C4-N3	3.29	119.76	114.84
1	A	34	CFZ	C3'-C2'-C1'	3.29	107.11	103.13
1	A	383	CFZ	C2'-C3'-C4'	3.29	106.66	102.40
1	A	334	UFT	C3'-C2'-C1'	3.29	107.11	103.13
1	A	26	CFZ	C3'-C2'-C1'	3.29	107.11	103.13
1	B	458	CFZ	C3'-C2'-C1'	3.29	107.11	103.13
1	B	94	UFT	C3'-C2'-C1'	3.29	107.11	103.13
1	A	212	CFZ	C3'-C2'-C1'	3.29	107.11	103.13
1	B	32	UFT	C5-C4-N3	3.29	119.75	114.84
1	B	620	CFZ	C2'-C3'-C4'	3.28	106.65	102.40
1	B	135	UFT	C5-C4-N3	3.28	119.75	114.84
1	B	10	CFZ	C2'-C3'-C4'	3.28	106.64	102.40
1	A	322	UFT	C5-C4-N3	3.28	119.75	114.84
1	A	682	CFZ	C2'-C1'-N1	-3.28	109.18	114.20
1	A	142	UFT	C3'-C2'-C1'	3.28	107.10	103.13
1	B	519	UFT	C3'-C2'-C1'	3.28	107.10	103.13
1	B	418	CFZ	C3'-C2'-C1'	3.28	107.10	103.13
1	A	635	UFT	C3'-C2'-C1'	3.28	107.10	103.13
1	A	315	CFZ	C2'-C3'-C4'	3.28	106.64	102.40
1	A	659	UFT	C5-C4-N3	3.28	119.75	114.84
1	A	418	CFZ	C3'-C2'-C1'	3.28	107.10	103.13
1	B	42	UFT	C5-C4-N3	3.28	119.75	114.84
1	B	142	UFT	C3'-C2'-C1'	3.28	107.10	103.13
1	B	196	UFT	C3'-C2'-C1'	3.28	107.10	103.13
1	B	431	UFT	C2'-C3'-C4'	3.28	106.64	102.40
1	B	196	UFT	C2'-C3'-C4'	3.28	106.64	102.40
1	A	437	UFT	C3'-C2'-C1'	3.27	107.09	103.13
1	B	234	CFZ	C2'-C3'-C4'	3.27	106.63	102.40
1	B	635	UFT	C2'-C3'-C4'	3.27	106.63	102.40
1	B	103	CFZ	C3'-C2'-C1'	3.27	107.09	103.13
1	B	437	UFT	C3'-C2'-C1'	3.27	107.09	103.13
1	A	691	CFZ	C3'-C2'-C1'	3.27	107.08	103.13
1	B	67	CFZ	C2'-C3'-C4'	3.27	106.62	102.40
1	A	97	UFT	C3'-C2'-C1'	3.27	107.08	103.13
1	A	358	UFT	C5-C4-N3	3.26	119.72	114.84
1	A	218	CFZ	C3'-C2'-C1'	3.26	107.08	103.13
1	B	72	CFZ	C2'-C1'-N1	-3.26	109.22	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	372	CFZ	C3'-C2'-C1'	3.26	107.08	103.13
1	A	335	CFZ	C2'-C3'-C4'	3.26	106.61	102.40
1	B	26	CFZ	C3'-C2'-C1'	3.26	107.08	103.13
1	B	403	UFT	C3'-C2'-C1'	3.26	107.08	103.13
1	A	50	UFT	C2'-C1'-N1	-3.26	109.22	114.20
1	B	73	CFZ	C2'-C1'-N1	-3.26	109.22	114.20
1	A	214	UFT	C3'-C2'-C1'	3.25	107.07	103.13
1	B	369	CFZ	C3'-C2'-C1'	3.25	107.07	103.13
1	B	590	UFT	C3'-C2'-C1'	3.25	107.07	103.13
1	B	554	UFT	C3'-C2'-C1'	3.25	107.07	103.13
1	B	164	CFZ	C3'-C2'-C1'	3.25	107.07	103.13
1	B	691	CFZ	C3'-C2'-C1'	3.25	107.07	103.13
1	A	524	UFT	C5-C4-N3	3.25	119.70	114.84
1	A	491	CFZ	C3'-C2'-C1'	3.25	107.06	103.13
1	A	196	UFT	C2'-C3'-C4'	3.25	106.60	102.40
1	B	161	CFZ	C3'-C2'-C1'	3.25	107.06	103.13
1	B	682	CFZ	C2'-C1'-N1	-3.25	109.24	114.20
1	B	720	UFT	C5-C4-N3	3.25	119.70	114.84
1	B	607	UFT	C2'-C3'-C4'	3.24	106.59	102.40
1	B	656	UFT	C2'-C3'-C4'	3.24	106.59	102.40
1	B	399	CFZ	C3'-C2'-C1'	3.24	107.06	103.13
1	A	576	CFZ	C3'-C2'-C1'	3.24	107.06	103.13
1	A	196	UFT	C3'-C2'-C1'	3.24	107.06	103.13
1	A	197	UFT	C3'-C2'-C1'	3.24	107.05	103.13
1	B	115	UFT	C3'-C2'-C1'	3.24	107.05	103.13
1	A	96	CFZ	C2'-C3'-C4'	3.23	106.58	102.40
1	A	635	UFT	C2'-C3'-C4'	3.23	106.58	102.40
1	A	458	CFZ	C3'-C2'-C1'	3.23	107.04	103.13
1	A	161	CFZ	C3'-C2'-C1'	3.23	107.04	103.13
1	B	430	UFT	C3'-C2'-C1'	3.23	107.04	103.13
1	B	635	UFT	C3'-C2'-C1'	3.23	107.04	103.13
1	A	115	UFT	C3'-C2'-C1'	3.23	107.04	103.13
1	A	214	UFT	C5-C4-N3	3.23	119.67	114.84
1	B	165	CFZ	C2'-C1'-N1	-3.23	109.27	114.20
1	B	232	CFZ	C2'-C3'-C4'	3.23	106.57	102.40
1	A	165	CFZ	C2'-C1'-N1	-3.23	109.27	114.20
1	A	399	CFZ	C3'-C2'-C1'	3.23	107.04	103.13
1	A	676	UFT	C2'-C3'-C4'	3.23	106.57	102.40
1	B	667	CFZ	C3'-C2'-C1'	3.22	107.03	103.13
1	A	283	UFT	C2'-C1'-N1	-3.22	109.27	114.20
1	B	216	UFT	C5-C4-N3	3.22	119.66	114.84
1	A	430	UFT	C3'-C2'-C1'	3.22	107.03	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	UFT	C2'-C3'-C4'	3.22	106.57	102.40
1	B	473	CFZ	C2'-C3'-C4'	3.22	106.57	102.40
1	B	296	UFT	C3'-C2'-C1'	3.22	107.03	103.13
1	B	506	CFZ	C3'-C2'-C1'	3.22	107.03	103.13
1	B	465	CFZ	C3'-C2'-C1'	3.22	107.03	103.13
1	A	43	UFT	C5-C4-N3	3.22	119.66	114.84
1	B	441	CFZ	C3'-C2'-C1'	3.22	107.03	103.13
1	B	218	CFZ	C2'-C3'-C4'	3.22	106.56	102.40
1	B	43	UFT	C5-C4-N3	3.22	119.65	114.84
1	A	72	CFZ	C3'-C2'-C1'	3.21	107.02	103.13
1	A	296	UFT	C3'-C2'-C1'	3.21	107.02	103.13
1	B	352	UFT	C3'-C2'-C1'	3.21	107.02	103.13
1	B	283	UFT	C2'-C1'-N1	-3.21	109.30	114.20
1	B	197	UFT	C3'-C2'-C1'	3.21	107.01	103.13
1	A	103	CFZ	C2'-C3'-C4'	3.21	106.55	102.40
1	A	465	CFZ	C3'-C2'-C1'	3.21	107.01	103.13
1	A	233	UFT	C3'-C2'-C1'	3.20	107.01	103.13
1	B	336	UFT	C3'-C2'-C1'	3.20	107.01	103.13
1	A	359	UFT	C5-C4-N3	3.20	119.63	114.84
1	B	486	CFZ	C2'-C3'-C4'	3.20	106.54	102.40
1	B	234	CFZ	C3'-C2'-C1'	3.20	107.00	103.13
1	A	361	UFT	C2'-C3'-C4'	3.20	106.53	102.40
1	B	704	CFZ	C3'-C2'-C1'	3.20	107.00	103.13
1	A	96	CFZ	C3'-C2'-C1'	3.19	106.99	103.13
1	A	518	CFZ	C2'-C3'-C4'	3.19	106.52	102.40
1	B	676	UFT	C2'-C3'-C4'	3.18	106.52	102.40
1	B	265	UFT	C3'-C2'-C1'	3.18	106.98	103.13
1	B	302	UFT	O4-C4-C5	-3.18	119.56	125.16
1	A	540	CFZ	C3'-C2'-C1'	3.18	106.98	103.13
1	B	530	UFT	C3'-C2'-C1'	3.18	106.98	103.13
1	A	61	UFT	C2'-C3'-C4'	3.17	106.50	102.40
1	A	139	CFZ	C3'-C2'-C1'	3.17	106.97	103.13
1	A	506	CFZ	C3'-C2'-C1'	3.17	106.97	103.13
1	B	559	UFT	C3'-C2'-C1'	3.17	106.97	103.13
1	B	481	UFT	C2'-C3'-C4'	3.17	106.50	102.40
1	B	581	UFT	C3'-C2'-C1'	3.17	106.97	103.13
1	A	667	CFZ	C3'-C2'-C1'	3.17	106.97	103.13
1	A	481	UFT	C2'-C3'-C4'	3.17	106.50	102.40
1	B	215	UFT	C3'-C2'-C1'	3.17	106.97	103.13
1	A	581	UFT	C3'-C2'-C1'	3.17	106.97	103.13
1	B	430	UFT	C2'-C3'-C4'	3.17	106.50	102.40
1	B	426	CFZ	C2'-C1'-N1	-3.17	109.36	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	UFT	C2'-C3'-C4'	3.17	106.49	102.40
1	B	101	UFT	C3'-C2'-C1'	3.16	106.96	103.13
1	A	169	UFT	C2'-C3'-C4'	3.16	106.49	102.40
1	B	94	UFT	C2'-C3'-C4'	3.16	106.49	102.40
1	A	550	CFZ	C3'-C2'-C1'	3.16	106.96	103.13
1	B	358	UFT	C5-C4-N3	3.16	119.56	114.84
1	B	139	CFZ	C3'-C2'-C1'	3.16	106.95	103.13
1	A	302	UFT	O4-C4-C5	-3.16	119.61	125.16
1	B	106	UFT	C3'-C2'-C1'	3.16	106.95	103.13
1	A	592	CFZ	C2'-C1'-N1	-3.15	109.38	114.20
1	A	656	UFT	C2'-C3'-C4'	3.15	106.47	102.40
1	A	700	CFZ	C3'-C2'-C1'	3.15	106.94	103.13
1	B	106	UFT	C2'-C3'-C4'	3.15	106.47	102.40
1	A	106	UFT	C3'-C2'-C1'	3.15	106.94	103.13
1	A	704	CFZ	C3'-C2'-C1'	3.15	106.94	103.13
1	B	465	CFZ	C2'-C3'-C4'	3.15	106.47	102.40
1	A	464	UFT	C3'-C2'-C1'	3.15	106.94	103.13
1	A	352	UFT	C2'-C3'-C4'	3.15	106.47	102.40
1	B	242	CFZ	C3'-C2'-C1'	3.14	106.94	103.13
1	A	406	CFZ	C3'-C2'-C1'	3.14	106.94	103.13
1	A	426	CFZ	C2'-C1'-N1	-3.14	109.39	114.20
1	A	646	UFT	C2'-C3'-C4'	3.14	106.47	102.40
1	B	389	UFT	C2'-C1'-N1	-3.14	109.40	114.20
1	B	485	UFT	C3'-C2'-C1'	3.14	106.93	103.13
1	B	405	CFZ	C3'-C2'-C1'	3.14	106.93	103.13
1	B	202	UFT	C2'-C3'-C4'	3.13	106.45	102.40
1	B	184	CFZ	C2'-C1'-N1	-3.13	109.41	114.20
1	A	106	UFT	C2'-C3'-C4'	3.13	106.44	102.40
1	B	103	CFZ	C2'-C3'-C4'	3.13	106.44	102.40
1	B	593	UFT	C3'-C2'-C1'	3.13	106.92	103.13
1	B	543	CFZ	C3'-C2'-C1'	3.12	106.91	103.13
1	A	79	CFZ	C2'-C3'-C4'	3.12	106.44	102.40
1	B	156	CFZ	C3'-C2'-C1'	3.12	106.91	103.13
1	A	332	CFZ	C3'-C2'-C1'	3.12	106.90	103.13
1	B	61	UFT	C2'-C3'-C4'	3.12	106.43	102.40
1	A	465	CFZ	C2'-C3'-C4'	3.12	106.43	102.40
1	A	73	CFZ	C2'-C1'-N1	-3.12	109.44	114.20
1	B	201	CFZ	C2'-C3'-C4'	3.11	106.43	102.40
1	B	424	CFZ	C3'-C2'-C1'	3.11	106.90	103.13
1	B	651	CFZ	C3'-C2'-C1'	3.11	106.90	103.13
1	A	129	CFZ	C2'-C1'-N1	-3.11	109.44	114.20
1	A	489	UFT	C3'-C2'-C1'	3.11	106.90	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	UFT	C2'-C3'-C4'	3.11	106.42	102.40
1	B	249	CFZ	C2'-C1'-N1	-3.11	109.45	114.20
1	A	543	CFZ	C3'-C2'-C1'	3.11	106.89	103.13
1	A	551	CFZ	C2'-C1'-N1	-3.11	109.45	114.20
1	B	512	CFZ	C2'-C1'-N1	-3.11	109.45	114.20
1	B	406	CFZ	C3'-C2'-C1'	3.11	106.89	103.13
1	A	98	UFT	O4-C4-C5	-3.11	119.70	125.16
1	A	336	UFT	C3'-C2'-C1'	3.11	106.89	103.13
1	A	608	UFT	C2'-C3'-C4'	3.10	106.42	102.40
1	B	646	UFT	C2'-C3'-C4'	3.10	106.42	102.40
1	B	332	CFZ	C3'-C2'-C1'	3.10	106.89	103.13
1	B	129	CFZ	C2'-C1'-N1	-3.10	109.46	114.20
1	A	265	UFT	C3'-C2'-C1'	3.10	106.89	103.13
1	B	592	CFZ	C2'-C1'-N1	-3.10	109.46	114.20
1	B	434	UFT	C2'-C3'-C4'	3.10	106.41	102.40
1	A	689	UFT	C2'-C3'-C4'	3.10	106.41	102.40
1	A	206	CFZ	C2'-C3'-C4'	3.09	106.40	102.40
1	A	372	CFZ	C2'-C3'-C4'	3.09	106.40	102.40
1	A	424	CFZ	C3'-C2'-C1'	3.09	106.88	103.13
1	A	708	UFT	C2'-C1'-N1	-3.09	109.47	114.20
1	B	700	CFZ	C3'-C2'-C1'	3.09	106.87	103.13
1	B	217	UFT	C3'-C2'-C1'	3.09	106.87	103.13
1	A	115	UFT	C2'-C3'-C4'	3.09	106.40	102.40
1	A	405	CFZ	C3'-C2'-C1'	3.09	106.87	103.13
1	A	184	CFZ	C2'-C1'-N1	-3.09	109.48	114.20
1	B	197	UFT	C2'-C3'-C4'	3.09	106.39	102.40
1	B	708	UFT	C2'-C1'-N1	-3.09	109.48	114.20
1	A	351	CFZ	C3'-C2'-C1'	3.08	106.86	103.13
1	B	464	UFT	C2'-C3'-C4'	3.08	106.39	102.40
1	B	347	UFT	C3'-C2'-C1'	3.08	106.86	103.13
1	A	434	UFT	C2'-C3'-C4'	3.08	106.38	102.40
1	A	164	CFZ	C3'-C2'-C1'	3.08	106.86	103.13
1	A	197	UFT	C2'-C3'-C4'	3.08	106.38	102.40
1	A	460	UFT	C2'-C1'-N1	-3.08	109.50	114.20
1	B	554	UFT	C2'-C3'-C4'	3.07	106.38	102.40
1	B	633	UFT	C2'-C1'-N1	-3.07	109.50	114.20
1	A	156	CFZ	C3'-C2'-C1'	3.07	106.85	103.13
1	B	662	UFT	C3'-C2'-C1'	3.07	106.85	103.13
1	A	639	CFZ	C3'-C2'-C1'	3.07	106.85	103.13
1	B	548	CFZ	C2'-C3'-C4'	3.07	106.37	102.40
1	A	451	CFZ	C3'-C2'-C1'	3.07	106.84	103.13
1	B	460	UFT	C2'-C1'-N1	-3.07	109.51	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	UFT	C2'-C3'-C4'	3.06	106.36	102.40
1	A	581	UFT	C2'-C3'-C4'	3.06	106.36	102.40
1	A	511	CFZ	C3'-C2'-C1'	3.06	106.84	103.13
1	A	651	CFZ	C3'-C2'-C1'	3.06	106.84	103.13
1	B	115	UFT	C2'-C3'-C4'	3.06	106.36	102.40
1	B	372	CFZ	C2'-C3'-C4'	3.06	106.36	102.40
1	A	232	CFZ	C3'-C2'-C1'	3.06	106.83	103.13
1	B	696	UFT	C3'-C2'-C1'	3.06	106.83	103.13
1	A	249	CFZ	C2'-C1'-N1	-3.06	109.53	114.20
1	B	98	UFT	C2'-C1'-N1	-3.06	109.53	114.20
1	A	157	CFZ	C2'-C1'-N1	-3.06	109.53	114.20
1	A	266	UFT	C2'-C3'-C4'	3.06	106.35	102.40
1	B	703	UFT	C2'-C1'-N1	-3.06	109.53	114.20
1	A	160	UFT	C2'-C3'-C4'	3.05	106.35	102.40
1	B	689	UFT	C2'-C3'-C4'	3.05	106.35	102.40
1	B	266	UFT	C2'-C3'-C4'	3.05	106.35	102.40
1	B	494	CFZ	C3'-C2'-C1'	3.05	106.83	103.13
1	B	387	CFZ	C2'-C1'-N1	-3.05	109.54	114.20
1	A	494	CFZ	C3'-C2'-C1'	3.05	106.83	103.13
1	B	425	CFZ	C3'-C2'-C1'	3.05	106.82	103.13
1	A	21	CFZ	C3'-C2'-C1'	3.05	106.82	103.13
1	B	142	UFT	C2'-C3'-C4'	3.05	106.34	102.40
1	A	662	UFT	C3'-C2'-C1'	3.05	106.82	103.13
1	A	632	CFZ	C2'-C3'-C4'	3.05	106.34	102.40
1	B	325	CFZ	C2'-C3'-C4'	3.05	106.34	102.40
1	B	550	CFZ	C3'-C2'-C1'	3.05	106.82	103.13
1	A	548	CFZ	C3'-C2'-C1'	3.04	106.82	103.13
1	A	633	UFT	C2'-C1'-N1	-3.04	109.55	114.20
1	A	216	UFT	C5-C4-N3	3.04	119.39	114.84
1	B	383	CFZ	C3'-C2'-C1'	3.04	106.81	103.13
1	A	639	CFZ	C2'-C3'-C4'	3.04	106.33	102.40
1	A	404	CFZ	C3'-C2'-C1'	3.04	106.81	103.13
1	A	354	CFZ	C2'-C1'-N1	-3.04	109.56	114.20
1	A	464	UFT	C2'-C3'-C4'	3.04	106.33	102.40
1	B	667	CFZ	C2'-C3'-C4'	3.04	106.33	102.40
1	A	696	UFT	C3'-C2'-C1'	3.04	106.81	103.13
1	B	206	CFZ	C2'-C3'-C4'	3.04	106.33	102.40
1	B	265	UFT	C2'-C3'-C4'	3.04	106.33	102.40
1	A	142	UFT	C2'-C3'-C4'	3.04	106.33	102.40
1	A	350	UFT	O4-C4-C5	-3.03	119.82	125.16
1	B	201	CFZ	C3'-C2'-C1'	3.03	106.81	103.13
1	B	229	UFT	C2'-C1'-N1	-3.03	109.56	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	581	UFT	C2'-C3'-C4'	3.03	106.32	102.40
1	A	242	CFZ	C3'-C2'-C1'	3.03	106.80	103.13
1	A	625	CFZ	C2'-C3'-C4'	3.03	106.32	102.40
1	B	639	CFZ	C2'-C3'-C4'	3.03	106.32	102.40
1	A	666	UFT	C3'-C2'-C1'	3.03	106.80	103.13
1	B	44	UFT	O4-C4-C5	-3.03	119.84	125.16
1	B	625	CFZ	C2'-C3'-C4'	3.03	106.31	102.40
1	B	404	CFZ	C3'-C2'-C1'	3.03	106.79	103.13
1	A	436	CFZ	C3'-C2'-C1'	3.02	106.79	103.13
1	A	151	CFZ	C2'-C3'-C4'	3.02	106.31	102.40
1	B	173	CFZ	C3'-C2'-C1'	3.02	106.79	103.13
1	A	352	UFT	O4-C4-C5	-3.02	119.85	125.16
1	B	43	UFT	C3'-C2'-C1'	3.02	106.78	103.13
1	A	543	CFZ	C2'-C3'-C4'	3.02	106.30	102.40
1	B	84	UFT	C2'-C3'-C4'	3.02	106.30	102.40
1	B	104	CFZ	C2'-C1'-N1	-3.02	109.59	114.20
1	A	549	UFT	C3'-C2'-C1'	3.02	106.78	103.13
1	B	160	UFT	C2'-C3'-C4'	3.02	106.30	102.40
1	A	602	UFT	C2'-C1'-N1	-3.01	109.59	114.20
1	B	548	CFZ	C3'-C2'-C1'	3.01	106.78	103.13
1	A	201	CFZ	C3'-C2'-C1'	3.01	106.78	103.13
1	B	151	CFZ	C2'-C3'-C4'	3.01	106.30	102.40
1	B	440	CFZ	C3'-C2'-C1'	3.01	106.78	103.13
1	B	79	CFZ	C2'-C3'-C4'	3.01	106.29	102.40
1	B	571	UFT	C2'-C3'-C4'	3.01	106.29	102.40
1	B	719	UFT	O4-C4-C5	-3.01	119.87	125.16
1	A	215	UFT	C5-C4-N3	3.01	119.34	114.84
1	A	703	UFT	C2'-C1'-N1	-3.01	109.61	114.20
1	B	361	UFT	O4-C4-C5	-3.00	119.88	125.16
1	A	481	UFT	C3'-C2'-C1'	3.00	106.77	103.13
1	A	540	CFZ	C2'-C3'-C4'	3.00	106.28	102.40
1	A	693	CFZ	C2'-C1'-N1	-3.00	109.61	114.20
1	B	632	CFZ	C2'-C3'-C4'	3.00	106.28	102.40
1	B	540	CFZ	C3'-C2'-C1'	3.00	106.76	103.13
1	A	44	UFT	O4-C4-C5	-3.00	119.89	125.16
1	A	554	UFT	C3'-C2'-C1'	3.00	106.76	103.13
1	A	426	CFZ	C3'-C2'-C1'	3.00	106.76	103.13
1	A	559	UFT	C2'-C3'-C4'	3.00	106.28	102.40
1	B	492	CFZ	C2'-C1'-N1	-3.00	109.62	114.20
1	B	432	UFT	O4-C4-C5	-3.00	119.89	125.16
1	B	254	CFZ	C2'-C1'-N1	-2.99	109.62	114.20
1	B	157	CFZ	C2'-C1'-N1	-2.99	109.62	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	639	CFZ	C3'-C2'-C1'	2.99	106.75	103.13
1	A	323	CFZ	C2'-C3'-C4'	2.99	106.27	102.40
1	A	321	CFZ	C2'-C1'-N1	-2.99	109.63	114.20
1	A	542	UFT	C3'-C2'-C1'	2.99	106.75	103.13
1	B	313	UFT	O4-C4-C5	-2.99	119.90	125.16
1	B	698	CFZ	C2'-C1'-N1	-2.99	109.63	114.20
1	A	577	UFT	C2'-C1'-N1	-2.99	109.63	114.20
1	A	384	CFZ	C2'-C3'-C4'	2.99	106.27	102.40
1	B	32	UFT	C3'-C2'-C1'	2.99	106.75	103.13
1	A	701	UFT	C2'-C3'-C4'	2.99	106.26	102.40
1	B	302	UFT	C2'-C3'-C4'	2.99	106.26	102.40
1	B	559	UFT	C2'-C3'-C4'	2.99	106.26	102.40
1	B	666	UFT	C3'-C2'-C1'	2.99	106.75	103.13
1	B	198	CFZ	C3'-C2'-C1'	2.98	106.74	103.13
1	A	485	UFT	C3'-C2'-C1'	2.98	106.74	103.13
1	A	447	UFT	C2'-C1'-N1	-2.98	109.64	114.20
1	B	108	UFT	C2'-C1'-N1	-2.98	109.64	114.20
1	A	60	UFT	O4-C4-C5	-2.98	119.92	125.16
1	A	360	CFZ	C2'-C3'-C4'	2.98	106.26	102.40
1	A	455	CFZ	C3'-C2'-C1'	2.98	106.74	103.13
1	A	101	UFT	O4-C4-C5	-2.98	119.92	125.16
1	B	571	UFT	C3'-C2'-C1'	2.98	106.74	103.13
1	B	98	UFT	O4-C4-C5	-2.98	119.92	125.16
1	A	432	UFT	O4-C4-C5	-2.98	119.92	125.16
1	B	398	UFT	C3'-C2'-C1'	2.98	106.73	103.13
1	A	571	UFT	C2'-C3'-C4'	2.97	106.25	102.40
1	B	359	UFT	C2'-C1'-N1	-2.97	109.65	114.20
1	A	667	CFZ	C2'-C3'-C4'	2.97	106.25	102.40
1	A	571	UFT	O4-C4-C5	-2.97	119.93	125.16
1	B	524	UFT	O4-C4-C5	-2.97	119.93	125.16
1	B	519	UFT	C2'-C3'-C4'	2.97	106.24	102.40
1	B	169	UFT	O4-C4-C5	-2.97	119.94	125.16
1	A	44	UFT	C2'-C1'-N1	-2.97	109.66	114.20
1	B	693	CFZ	C2'-C1'-N1	-2.97	109.66	114.20
1	B	542	UFT	C3'-C2'-C1'	2.97	106.73	103.13
1	A	548	CFZ	C2'-C3'-C4'	2.97	106.24	102.40
1	A	229	UFT	O4-C4-C5	-2.97	119.94	125.16
1	B	458	CFZ	C2'-C3'-C4'	2.97	106.24	102.40
1	A	618	UFT	O4-C4-C5	-2.97	119.94	125.16
1	B	509	UFT	C3'-C2'-C1'	2.97	106.72	103.13
1	A	334	UFT	O4-C4-C5	-2.97	119.94	125.16
1	B	217	UFT	O4-C4-C5	-2.97	119.94	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	UFT	C3'-C2'-C1'	2.97	106.72	103.13
1	B	426	CFZ	C3'-C2'-C1'	2.96	106.72	103.13
1	B	69	UFT	O4-C4-C5	-2.96	119.95	125.16
1	A	437	UFT	O4-C4-C5	-2.96	119.95	125.16
1	A	698	CFZ	C2'-C1'-N1	-2.96	109.67	114.20
1	A	108	UFT	C2'-C1'-N1	-2.96	109.67	114.20
1	B	447	UFT	C2'-C1'-N1	-2.96	109.67	114.20
1	A	647	CFZ	C3'-C2'-C1'	2.96	106.72	103.13
1	A	55	UFT	O4-C4-C5	-2.96	119.95	125.16
1	B	182	UFT	O4-C4-C5	-2.96	119.95	125.16
1	A	471	UFT	O4-C4-C5	-2.96	119.96	125.16
1	A	509	UFT	C3'-C2'-C1'	2.96	106.71	103.13
1	A	493	UFT	O4-C4-C5	-2.96	119.96	125.16
1	A	447	UFT	O4-C4-C5	-2.96	119.96	125.16
1	A	217	UFT	O4-C4-C5	-2.96	119.96	125.16
1	A	549	UFT	O4-C4-C5	-2.96	119.96	125.16
1	A	135	UFT	C2'-C3'-C4'	2.96	106.22	102.40
1	A	59	UFT	C3'-C2'-C1'	2.95	106.71	103.13
1	B	62	UFT	O4-C4-C5	-2.95	119.96	125.16
1	A	283	UFT	O4-C4-C5	-2.95	119.97	125.16
1	A	305	UFT	O4-C4-C5	-2.95	119.97	125.16
1	A	720	UFT	C3'-C2'-C1'	2.95	106.71	103.13
1	A	719	UFT	O4-C4-C5	-2.95	119.97	125.16
1	B	543	CFZ	C2'-C3'-C4'	2.95	106.22	102.40
1	B	587	CFZ	C2'-C1'-N1	-2.95	109.69	114.20
1	B	481	UFT	C3'-C2'-C1'	2.95	106.70	103.13
1	B	92	UFT	O4-C4-C5	-2.95	119.97	125.16
1	B	635	UFT	O4-C4-C5	-2.95	119.97	125.16
1	B	179	UFT	C3'-C2'-C1'	2.95	106.70	103.13
1	B	559	UFT	O4-C4-C5	-2.95	119.97	125.16
1	B	618	UFT	O4-C4-C5	-2.95	119.97	125.16
1	B	530	UFT	C2'-C3'-C4'	2.95	106.22	102.40
1	B	456	UFT	O4-C4-C5	-2.95	119.97	125.16
1	A	628	UFT	O4-C4-C5	-2.95	119.97	125.16
1	B	204	UFT	O4-C4-C5	-2.95	119.97	125.16
1	A	43	UFT	C3'-C2'-C1'	2.95	106.70	103.13
1	A	216	UFT	C3'-C2'-C1'	2.95	106.70	103.13
1	A	425	CFZ	C3'-C2'-C1'	2.95	106.70	103.13
1	B	511	CFZ	C3'-C2'-C1'	2.95	106.70	103.13
1	B	329	UFT	C2'-C1'-N1	-2.95	109.69	114.20
1	B	156	CFZ	C2'-C3'-C4'	2.95	106.21	102.40
1	A	197	UFT	O4-C4-C5	-2.95	119.97	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	UFT	O4-C4-C5	-2.95	119.97	125.16
1	B	534	UFT	O4-C4-C5	-2.95	119.98	125.16
1	A	687	UFT	O4-C4-C5	-2.95	119.98	125.16
1	B	283	UFT	O4-C4-C5	-2.95	119.98	125.16
1	B	33	UFT	C3'-C2'-C1'	2.95	106.70	103.13
1	A	143	UFT	O4-C4-C5	-2.95	119.98	125.16
1	A	462	CFZ	C3'-C2'-C1'	2.95	106.70	103.13
1	A	142	UFT	O4-C4-C5	-2.95	119.98	125.16
1	B	344	UFT	O4-C4-C5	-2.95	119.98	125.16
1	A	656	UFT	O4-C4-C5	-2.95	119.98	125.16
1	A	182	UFT	O4-C4-C5	-2.95	119.98	125.16
1	B	609	UFT	O4-C4-C5	-2.95	119.98	125.16
1	B	44	UFT	C2'-C1'-N1	-2.94	109.70	114.20
1	A	712	UFT	O4-C4-C5	-2.94	119.98	125.16
1	B	71	UFT	O4-C4-C5	-2.94	119.98	125.16
1	A	170	UFT	O4-C4-C5	-2.94	119.98	125.16
1	B	61	UFT	O4-C4-C5	-2.94	119.98	125.16
1	B	430	UFT	O4-C4-C5	-2.94	119.99	125.16
1	A	635	UFT	O4-C4-C5	-2.94	119.99	125.16
1	B	659	UFT	C2'-C3'-C4'	2.94	106.20	102.40
1	B	549	UFT	C3'-C2'-C1'	2.94	106.69	103.13
1	A	204	UFT	O4-C4-C5	-2.94	119.99	125.16
1	A	309	UFT	O4-C4-C5	-2.94	119.99	125.16
1	A	643	CFZ	C2'-C1'-N1	-2.94	109.71	114.20
1	A	434	UFT	O4-C4-C5	-2.94	119.99	125.16
1	B	643	CFZ	C2'-C1'-N1	-2.94	109.71	114.20
1	A	500	UFT	O4-C4-C5	-2.94	119.99	125.16
1	B	606	UFT	O4-C4-C5	-2.94	119.99	125.16
1	B	608	UFT	O4-C4-C5	-2.94	119.99	125.16
1	A	160	UFT	O4-C4-C5	-2.94	120.00	125.16
1	B	545	UFT	O4-C4-C5	-2.94	120.00	125.16
1	A	666	UFT	O4-C4-C5	-2.94	120.00	125.16
1	A	695	UFT	O4-C4-C5	-2.94	120.00	125.16
1	A	155	UFT	O4-C4-C5	-2.94	120.00	125.16
1	B	437	UFT	O4-C4-C5	-2.94	120.00	125.16
1	B	577	UFT	O4-C4-C5	-2.94	120.00	125.16
1	B	628	UFT	O4-C4-C5	-2.94	120.00	125.16
1	A	329	UFT	C2'-C1'-N1	-2.94	109.71	114.20
1	B	89	UFT	O4-C4-C5	-2.94	120.00	125.16
1	B	421	UFT	O4-C4-C5	-2.94	120.00	125.16
1	A	49	CFZ	C2'-C1'-N1	-2.94	109.71	114.20
1	A	582	UFT	O4-C4-C5	-2.94	120.00	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	CFZ	C3'-C2'-C1'	2.93	106.68	103.13
1	A	84	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	88	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	92	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	251	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	398	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	464	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	84	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	155	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	456	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	471	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	86	UFT	C2'-C1'-N1	-2.93	109.72	114.20
1	B	712	UFT	C2'-C1'-N1	-2.93	109.72	114.20
1	A	11	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	61	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	197	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	545	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	472	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	687	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	50	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	169	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	662	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	104	CFZ	C2'-C1'-N1	-2.93	109.72	114.20
1	B	94	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	229	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	434	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	141	UFT	C2'-C3'-C4'	2.93	106.19	102.40
1	B	265	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	549	UFT	O4-C4-C5	-2.93	120.00	125.16
1	B	582	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	663	UFT	O4-C4-C5	-2.93	120.00	125.16
1	A	509	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	305	UFT	C3'-C2'-C1'	2.93	106.68	103.13
1	A	201	CFZ	C2'-C3'-C4'	2.93	106.19	102.40
1	A	97	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	708	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	499	UFT	C3'-C2'-C1'	2.93	106.68	103.13
1	A	209	CFZ	C2'-C1'-N1	-2.93	109.72	114.20
1	A	621	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	304	CFZ	C2'-C1'-N1	-2.93	109.72	114.20
1	A	568	CFZ	C2'-C1'-N1	-2.93	109.72	114.20
1	B	101	UFT	O4-C4-C5	-2.93	120.01	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	137	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	14	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	554	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	656	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	378	CFZ	C2'-C1'-N1	-2.93	109.72	114.20
1	A	94	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	126	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	174	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	398	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	593	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	636	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	378	CFZ	C2'-C1'-N1	-2.93	109.72	114.20
1	B	701	UFT	C2'-C3'-C4'	2.93	106.19	102.40
1	B	112	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	216	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	266	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	464	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	80	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	293	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	472	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	708	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	398	UFT	C3'-C2'-C1'	2.93	106.67	103.13
1	A	245	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	447	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	519	UFT	O4-C4-C5	-2.93	120.01	125.16
1	B	571	UFT	O4-C4-C5	-2.93	120.01	125.16
1	A	403	UFT	C2'-C3'-C4'	2.93	106.18	102.40
1	B	120	CFZ	C3'-C2'-C1'	2.93	106.67	103.13
1	B	305	UFT	C3'-C2'-C1'	2.93	106.67	103.13
1	B	293	UFT	O4-C4-C5	-2.93	120.02	125.16
1	B	621	UFT	O4-C4-C5	-2.93	120.02	125.16
1	B	633	UFT	O4-C4-C5	-2.93	120.02	125.16
1	A	696	UFT	O4-C4-C5	-2.93	120.02	125.16
1	B	106	UFT	O4-C4-C5	-2.93	120.02	125.16
1	A	190	UFT	O4-C4-C5	-2.93	120.02	125.16
1	A	329	UFT	O4-C4-C5	-2.93	120.02	125.16
1	A	606	UFT	O4-C4-C5	-2.93	120.02	125.16
1	A	112	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	530	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	296	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	590	UFT	O4-C4-C5	-2.92	120.02	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	CFZ	C2'-C1'-N1	-2.92	109.73	114.20
1	B	212	CFZ	C2'-C3'-C4'	2.92	106.18	102.40
1	A	86	UFT	O4-C4-C5	-2.92	120.02	125.16
1	B	143	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	270	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	430	UFT	O4-C4-C5	-2.92	120.02	125.16
1	B	190	UFT	O4-C4-C5	-2.92	120.02	125.16
1	B	192	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	504	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	98	UFT	C2'-C1'-N1	-2.92	109.73	114.20
1	A	89	UFT	O4-C4-C5	-2.92	120.02	125.16
1	B	653	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	8	UFT	O4-C4-C5	-2.92	120.02	125.16
1	B	504	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	559	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	646	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	14	UFT	C2'-C1'-N1	-2.92	109.74	114.20
1	A	137	UFT	O4-C4-C5	-2.92	120.02	125.16
1	B	208	UFT	O4-C4-C5	-2.92	120.02	125.16
1	A	265	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	14	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	609	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	293	UFT	C2'-C1'-N1	-2.92	109.74	114.20
1	A	503	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	653	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	662	UFT	O4-C4-C5	-2.92	120.03	125.16
1	B	712	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	302	UFT	C2'-C3'-C4'	2.92	106.17	102.40
1	A	115	UFT	O4-C4-C5	-2.92	120.03	125.16
1	B	423	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	689	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	155	UFT	C3'-C2'-C1'	2.92	106.66	103.13
1	B	647	CFZ	C3'-C2'-C1'	2.92	106.66	103.13
1	A	179	UFT	O4-C4-C5	-2.92	120.03	125.16
1	B	509	UFT	O4-C4-C5	-2.92	120.03	125.16
1	B	530	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	74	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	154	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	499	UFT	O4-C4-C5	-2.92	120.03	125.16
1	B	163	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	519	UFT	O4-C4-C5	-2.92	120.03	125.16
1	A	633	UFT	O4-C4-C5	-2.92	120.03	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	UFT	O4-C4-C5	-2.92	120.03	125.16
1	B	377	UFT	O4-C4-C5	-2.92	120.03	125.16
1	B	502	UFT	O4-C4-C5	-2.92	120.03	125.16
1	B	669	UFT	O4-C4-C5	-2.92	120.03	125.16
1	B	19	UFT	O4-C4-C5	-2.91	120.03	125.16
1	A	106	UFT	O4-C4-C5	-2.91	120.03	125.16
1	B	141	UFT	O4-C4-C5	-2.91	120.03	125.16
1	B	170	UFT	O4-C4-C5	-2.91	120.03	125.16
1	A	200	UFT	O4-C4-C5	-2.91	120.03	125.16
1	B	663	UFT	O4-C4-C5	-2.91	120.03	125.16
1	B	689	UFT	O4-C4-C5	-2.91	120.03	125.16
1	A	585	CFZ	C2'-C1'-N1	-2.91	109.75	114.20
1	A	202	UFT	O4-C4-C5	-2.91	120.03	125.16
1	A	460	UFT	O4-C4-C5	-2.91	120.03	125.16
1	B	74	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	116	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	163	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	296	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	344	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	424	CFZ	C2'-C3'-C4'	2.91	106.17	102.40
1	A	135	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	305	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	466	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	500	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	502	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	534	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	11	UFT	C3'-C2'-C1'	2.91	106.66	103.13
1	A	71	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	554	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	309	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	97	UFT	C3'-C2'-C1'	2.91	106.66	103.13
1	B	59	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	214	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	423	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	695	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	32	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	389	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	403	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	555	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	673	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	198	CFZ	C3'-C2'-C1'	2.91	106.65	103.13
1	B	215	UFT	O4-C4-C5	-2.91	120.04	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	361	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	366	UFT	O4-C4-C5	-2.91	120.04	125.16
1	A	485	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	154	UFT	O4-C4-C5	-2.91	120.04	125.16
1	B	141	UFT	C2'-C3'-C4'	2.91	106.16	102.40
1	B	43	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	192	UFT	O4-C4-C5	-2.91	120.05	125.16
1	B	402	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	577	UFT	O4-C4-C5	-2.91	120.05	125.16
1	B	646	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	474	CFZ	C3'-C2'-C1'	2.91	106.65	103.13
1	B	301	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	542	UFT	O4-C4-C5	-2.91	120.05	125.16
1	B	13	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	175	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	208	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	88	UFT	O4-C4-C5	-2.91	120.05	125.16
1	B	116	UFT	O4-C4-C5	-2.91	120.05	125.16
1	B	200	UFT	O4-C4-C5	-2.91	120.05	125.16
1	B	636	UFT	O4-C4-C5	-2.91	120.05	125.16
1	B	55	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	266	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	581	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	108	UFT	O4-C4-C5	-2.91	120.05	125.16
1	B	629	UFT	O4-C4-C5	-2.91	120.05	125.16
1	B	696	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	413	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	684	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	690	UFT	O4-C4-C5	-2.91	120.05	125.16
1	A	512	CFZ	C2'-C1'-N1	-2.91	109.76	114.20
1	A	48	UFT	O4-C4-C5	-2.90	120.05	125.16
1	A	59	UFT	O4-C4-C5	-2.90	120.05	125.16
1	B	153	UFT	O4-C4-C5	-2.90	120.05	125.16
1	B	179	UFT	O4-C4-C5	-2.90	120.05	125.16
1	B	251	UFT	O4-C4-C5	-2.90	120.05	125.16
1	A	336	UFT	O4-C4-C5	-2.90	120.05	125.16
1	B	336	UFT	O4-C4-C5	-2.90	120.05	125.16
1	A	377	UFT	O4-C4-C5	-2.90	120.05	125.16
1	A	555	UFT	O4-C4-C5	-2.90	120.05	125.16
1	A	720	UFT	O4-C4-C5	-2.90	120.05	125.16
1	A	402	UFT	O4-C4-C5	-2.90	120.06	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	673	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	60	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	629	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	458	CFZ	C2'-C3'-C4'	2.90	106.15	102.40
1	B	581	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	701	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	43	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	62	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	293	UFT	C2'-C1'-N1	-2.90	109.77	114.20
1	A	13	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	466	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	142	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	50	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	607	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	141	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	174	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	322	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	602	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	69	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	403	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	481	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	421	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	155	UFT	C3'-C2'-C1'	2.90	106.64	103.13
1	B	105	UFT	C1'-N1-C2	2.90	122.82	117.57
1	B	607	UFT	O4-C4-C5	-2.90	120.06	125.16
1	A	608	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	690	UFT	O4-C4-C5	-2.90	120.06	125.16
1	B	604	CFZ	C2'-C1'-N1	-2.90	109.77	114.20
1	A	266	UFT	C3'-C2'-C1'	2.90	106.64	103.13
1	B	175	UFT	O4-C4-C5	-2.90	120.07	125.16
1	A	233	UFT	O4-C4-C5	-2.90	120.07	125.16
1	A	485	UFT	C2'-C3'-C4'	2.90	106.14	102.40
1	A	602	UFT	O4-C4-C5	-2.90	120.07	125.16
1	B	329	UFT	O4-C4-C5	-2.90	120.07	125.16
1	B	108	UFT	O4-C4-C5	-2.89	120.07	125.16
1	A	260	UFT	O4-C4-C5	-2.89	120.07	125.16
1	A	347	UFT	O4-C4-C5	-2.89	120.07	125.16
1	A	720	UFT	C2'-C3'-C4'	2.89	106.14	102.40
1	A	365	UFT	O4-C4-C5	-2.89	120.07	125.16
1	B	684	UFT	O4-C4-C5	-2.89	120.07	125.16
1	B	140	CFZ	C2'-C3'-C4'	2.89	106.14	102.40
1	B	582	UFT	C2'-C1'-N1	-2.89	109.78	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	UFT	O4-C4-C5	-2.89	120.07	125.16
1	B	542	UFT	O4-C4-C5	-2.89	120.08	125.16
1	B	209	CFZ	C2'-C1'-N1	-2.89	109.78	114.20
1	B	233	UFT	O4-C4-C5	-2.89	120.08	125.16
1	B	160	UFT	O4-C4-C5	-2.89	120.08	125.16
1	A	703	UFT	O4-C4-C5	-2.89	120.08	125.16
1	A	373	CFZ	C3'-C2'-C1'	2.89	106.63	103.13
1	A	153	UFT	O4-C4-C5	-2.89	120.08	125.16
1	B	11	UFT	O4-C4-C5	-2.89	120.08	125.16
1	B	97	UFT	O4-C4-C5	-2.89	120.08	125.16
1	B	202	UFT	O4-C4-C5	-2.89	120.08	125.16
1	A	544	UFT	O4-C4-C5	-2.89	120.08	125.16
1	A	676	UFT	O4-C4-C5	-2.89	120.08	125.16
1	A	301	UFT	O4-C4-C5	-2.89	120.08	125.16
1	B	590	UFT	O4-C4-C5	-2.89	120.08	125.16
1	B	666	UFT	O4-C4-C5	-2.89	120.08	125.16
1	B	373	CFZ	C3'-C2'-C1'	2.89	106.63	103.13
1	B	460	UFT	O4-C4-C5	-2.89	120.08	125.16
1	B	481	UFT	O4-C4-C5	-2.89	120.08	125.16
1	A	669	UFT	O4-C4-C5	-2.89	120.08	125.16
1	A	367	UFT	O4-C4-C5	-2.89	120.08	125.16
1	A	556	CFZ	C2'-C3'-C4'	2.89	106.13	102.40
1	A	42	UFT	O4-C4-C5	-2.89	120.09	125.16
1	B	196	UFT	O4-C4-C5	-2.89	120.09	125.16
1	B	33	UFT	O4-C4-C5	-2.88	120.09	125.16
1	A	130	CFZ	C2'-C1'-N1	-2.88	109.79	114.20
1	A	247	CFZ	C2'-C1'-N1	-2.88	109.79	114.20
1	B	246	CFZ	C3'-C2'-C1'	2.88	106.62	103.13
1	B	579	CFZ	C3'-C2'-C1'	2.88	106.62	103.13
1	A	204	UFT	C2'-C3'-C4'	2.88	106.13	102.40
1	A	399	CFZ	C2'-C3'-C4'	2.88	106.13	102.40
1	A	593	UFT	C2'-C3'-C4'	2.88	106.13	102.40
1	B	8	UFT	O4-C4-C5	-2.88	120.09	125.16
1	A	105	UFT	O4-C4-C5	-2.88	120.09	125.16
1	A	196	UFT	O4-C4-C5	-2.88	120.09	125.16
1	A	366	UFT	O4-C4-C5	-2.88	120.09	125.16
1	A	431	UFT	O4-C4-C5	-2.88	120.09	125.16
1	B	659	UFT	O4-C4-C5	-2.88	120.09	125.16
1	B	695	UFT	C2'-C1'-N1	-2.88	109.79	114.20
1	B	270	UFT	O4-C4-C5	-2.88	120.09	125.16
1	A	254	CFZ	C2'-C1'-N1	-2.88	109.80	114.20
1	B	540	CFZ	C2'-C3'-C4'	2.88	106.13	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	657	CFZ	C2'-C3'-C4'	2.88	106.13	102.40
1	A	659	UFT	C2'-C3'-C4'	2.88	106.13	102.40
1	B	347	UFT	O4-C4-C5	-2.88	120.09	125.16
1	A	173	CFZ	C3'-C2'-C1'	2.88	106.62	103.13
1	B	135	UFT	C2'-C3'-C4'	2.88	106.12	102.40
1	B	260	UFT	O4-C4-C5	-2.88	120.10	125.16
1	B	365	UFT	O4-C4-C5	-2.88	120.10	125.16
1	B	485	UFT	O4-C4-C5	-2.88	120.10	125.16
1	A	585	CFZ	C3'-C2'-C1'	2.88	106.62	103.13
1	B	105	UFT	O4-C4-C5	-2.88	120.10	125.16
1	B	489	UFT	O4-C4-C5	-2.88	120.10	125.16
1	A	695	UFT	C2'-C1'-N1	-2.88	109.80	114.20
1	B	701	UFT	O4-C4-C5	-2.88	120.10	125.16
1	A	381	CFZ	C2'-C3'-C4'	2.88	106.12	102.40
1	A	32	UFT	O4-C4-C5	-2.88	120.10	125.16
1	B	474	CFZ	C2'-C1'-N1	-2.88	109.81	114.20
1	B	593	UFT	O4-C4-C5	-2.87	120.11	125.16
1	B	676	UFT	O4-C4-C5	-2.87	120.11	125.16
1	A	245	UFT	C3'-C2'-C1'	2.87	106.61	103.13
1	B	703	UFT	O4-C4-C5	-2.87	120.11	125.16
1	B	603	CFZ	C2'-C1'-N1	-2.87	109.81	114.20
1	B	266	UFT	C3'-C2'-C1'	2.87	106.61	103.13
1	B	604	CFZ	C3'-C2'-C1'	2.87	106.61	103.13
1	B	86	UFT	O4-C4-C5	-2.87	120.11	125.16
1	A	513	UFT	O4-C4-C5	-2.87	120.11	125.16
1	B	431	UFT	O4-C4-C5	-2.87	120.11	125.16
1	B	367	UFT	O4-C4-C5	-2.87	120.11	125.16
1	B	71	UFT	C3'-C2'-C1'	2.87	106.60	103.13
1	B	204	UFT	C2'-C3'-C4'	2.87	106.11	102.40
1	A	424	CFZ	C2'-C3'-C4'	2.87	106.11	102.40
1	B	130	CFZ	C2'-C1'-N1	-2.87	109.82	114.20
1	A	33	UFT	O4-C4-C5	-2.87	120.12	125.16
1	A	309	UFT	C3'-C2'-C1'	2.87	106.60	103.13
1	A	80	UFT	O4-C4-C5	-2.87	120.12	125.16
1	A	212	CFZ	C2'-C3'-C4'	2.86	106.11	102.40
1	B	582	UFT	C2'-C3'-C4'	2.86	106.11	102.40
1	A	19	UFT	O4-C4-C5	-2.86	120.12	125.16
1	A	582	UFT	C2'-C1'-N1	-2.86	109.82	114.20
1	B	216	UFT	O4-C4-C5	-2.86	120.12	125.16
1	A	140	CFZ	C2'-C3'-C4'	2.86	106.10	102.40
1	A	652	CFZ	C3'-C2'-C1'	2.86	106.60	103.13
1	B	389	UFT	O4-C4-C5	-2.86	120.13	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	UFT	O4-C4-C5	-2.86	120.13	125.16
1	B	504	UFT	C3'-C2'-C1'	2.86	106.59	103.13
1	B	39	CFZ	C2'-C1'-N1	-2.86	109.83	114.20
1	B	568	CFZ	C2'-C1'-N1	-2.86	109.83	114.20
1	A	163	UFT	C2'-C1'-N1	-2.86	109.83	114.20
1	B	163	UFT	C2'-C1'-N1	-2.86	109.83	114.20
1	B	336	UFT	C2'-C3'-C4'	2.86	106.09	102.40
1	A	494	CFZ	C2'-C3'-C4'	2.86	106.09	102.40
1	A	130	CFZ	C3'-C2'-C1'	2.86	106.59	103.13
1	B	245	UFT	O4-C4-C5	-2.86	120.14	125.16
1	A	603	CFZ	C2'-C1'-N1	-2.86	109.83	114.20
1	A	614	CFZ	C2'-C1'-N1	-2.86	109.83	114.20
1	B	405	CFZ	C2'-C3'-C4'	2.86	106.09	102.40
1	B	403	UFT	C2'-C3'-C4'	2.85	106.09	102.40
1	B	251	UFT	C2'-C1'-N1	-2.85	109.84	114.20
1	A	489	UFT	O4-C4-C5	-2.85	120.14	125.16
1	A	251	UFT	C2'-C1'-N1	-2.85	109.84	114.20
1	B	662	UFT	C2'-C3'-C4'	2.85	106.09	102.40
1	B	687	UFT	C2'-C1'-N1	-2.85	109.84	114.20
1	B	247	CFZ	C3'-C2'-C1'	2.85	106.58	103.13
1	B	474	CFZ	C3'-C2'-C1'	2.85	106.58	103.13
1	A	679	CFZ	C2'-C1'-N1	-2.85	109.84	114.20
1	B	378	CFZ	C3'-C2'-C1'	2.85	106.58	103.13
1	B	161	CFZ	C2'-C3'-C4'	2.85	106.08	102.40
1	B	84	UFT	C3'-C2'-C1'	2.85	106.58	103.13
1	B	689	UFT	C3'-C2'-C1'	2.85	106.58	103.13
1	A	587	CFZ	C2'-C1'-N1	-2.85	109.85	114.20
1	B	509	UFT	C2'-C3'-C4'	2.85	106.08	102.40
1	A	579	CFZ	C2'-C1'-N1	-2.85	109.85	114.20
1	B	544	UFT	O4-C4-C5	-2.85	120.15	125.16
1	A	659	UFT	O4-C4-C5	-2.85	120.15	125.16
1	A	509	UFT	C2'-C3'-C4'	2.85	106.08	102.40
1	A	313	UFT	O4-C4-C5	-2.85	120.16	125.16
1	A	679	CFZ	C3'-C2'-C1'	2.85	106.58	103.13
1	A	32	UFT	C3'-C2'-C1'	2.84	106.58	103.13
1	A	689	UFT	C3'-C2'-C1'	2.84	106.57	103.13
1	A	265	UFT	C2'-C3'-C4'	2.84	106.08	102.40
1	A	504	UFT	C3'-C2'-C1'	2.84	106.57	103.13
1	A	593	UFT	C3'-C2'-C1'	2.84	106.57	103.13
1	A	370	CFZ	C3'-C2'-C1'	2.84	106.57	103.13
1	A	137	UFT	C2'-C1'-N1	-2.84	109.86	114.20
1	B	130	CFZ	C3'-C2'-C1'	2.84	106.57	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	643	CFZ	C3'-C2'-C1'	2.84	106.57	103.13
1	B	659	UFT	C3'-C2'-C1'	2.84	106.57	103.13
1	A	418	CFZ	C2'-C1'-N1	-2.84	109.86	114.20
1	A	161	CFZ	C2'-C3'-C4'	2.84	106.07	102.40
1	B	173	CFZ	C2'-C3'-C4'	2.84	106.07	102.40
1	A	242	CFZ	C2'-C3'-C4'	2.84	106.07	102.40
1	B	370	CFZ	C2'-C3'-C4'	2.84	106.07	102.40
1	B	48	UFT	O4-C4-C5	-2.84	120.17	125.16
1	B	643	CFZ	C3'-C2'-C1'	2.83	106.56	103.13
1	B	325	CFZ	C3'-C2'-C1'	2.83	106.56	103.13
1	B	653	UFT	C3'-C2'-C1'	2.83	106.56	103.13
1	B	242	CFZ	C2'-C3'-C4'	2.83	106.06	102.40
1	A	219	CFZ	C2'-C1'-N1	-2.83	109.87	114.20
1	A	246	CFZ	C2'-C1'-N1	-2.83	109.87	114.20
1	B	352	UFT	O4-C4-C5	-2.83	120.18	125.16
1	A	405	CFZ	C2'-C3'-C4'	2.83	106.06	102.40
1	B	585	CFZ	C2'-C1'-N1	-2.83	109.87	114.20
1	B	720	UFT	O4-C4-C5	-2.83	120.18	125.16
1	A	378	CFZ	C3'-C2'-C1'	2.83	106.56	103.13
1	B	513	UFT	O4-C4-C5	-2.83	120.18	125.16
1	B	97	UFT	C2'-C3'-C4'	2.83	106.06	102.40
1	B	112	UFT	C3'-C2'-C1'	2.83	106.56	103.13
1	B	139	CFZ	C2'-C1'-N1	-2.83	109.88	114.20
1	A	451	CFZ	C2'-C1'-N1	-2.83	109.88	114.20
1	A	139	CFZ	C2'-C3'-C4'	2.83	106.06	102.40
1	B	164	CFZ	C2'-C3'-C4'	2.83	106.06	102.40
1	B	399	CFZ	C2'-C3'-C4'	2.83	106.06	102.40
1	A	407	CFZ	C3'-C2'-C1'	2.83	106.55	103.13
1	A	358	UFT	O4-C4-C5	-2.83	120.19	125.16
1	A	316	CFZ	C2'-C1'-N1	-2.83	109.88	114.20
1	B	363	CFZ	C2'-C1'-N1	-2.83	109.88	114.20
1	B	344	UFT	C2'-C1'-N1	-2.83	109.88	114.20
1	A	535	UFT	O4-C4-C5	-2.83	120.19	125.16
1	B	313	UFT	C2'-C1'-N1	-2.82	109.88	114.20
1	B	19	UFT	C2'-C3'-C4'	2.82	106.05	102.40
1	B	71	UFT	C2'-C3'-C4'	2.82	106.05	102.40
1	A	105	UFT	C2'-C3'-C4'	2.82	106.05	102.40
1	B	175	UFT	C2'-C3'-C4'	2.82	106.05	102.40
1	B	370	CFZ	C3'-C2'-C1'	2.82	106.55	103.13
1	B	323	CFZ	C3'-C2'-C1'	2.82	106.55	103.13
1	A	687	UFT	C2'-C1'-N1	-2.82	109.89	114.20
1	A	139	CFZ	C2'-C1'-N1	-2.82	109.89	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	652	CFZ	C3'-C2'-C1'	2.82	106.54	103.13
1	B	55	UFT	C2'-C1'-N1	-2.82	109.89	114.20
1	A	370	CFZ	C2'-C3'-C4'	2.81	106.04	102.40
1	A	486	CFZ	C4'-O4'-C1'	-2.81	103.26	109.47
1	A	322	UFT	O4-C4-C5	-2.81	120.21	125.16
1	B	105	UFT	C2'-C3'-C4'	2.81	106.04	102.40
1	A	366	UFT	C2'-C3'-C4'	2.81	106.04	102.40
1	B	574	CFZ	C2'-C1'-N1	-2.81	109.90	114.20
1	A	229	UFT	C2'-C3'-C4'	2.81	106.04	102.40
1	A	86	UFT	C2'-C1'-N1	-2.81	109.90	114.20
1	B	131	CFZ	C2'-C1'-N1	-2.81	109.90	114.20
1	B	302	UFT	C3'-C2'-C1'	2.81	106.53	103.13
1	B	316	CFZ	C2'-C1'-N1	-2.81	109.90	114.20
1	A	474	CFZ	C2'-C1'-N1	-2.81	109.90	114.20
1	A	105	UFT	C1'-N1-C2	2.81	122.66	117.57
1	B	219	CFZ	C2'-C1'-N1	-2.81	109.91	114.20
1	A	88	UFT	C3'-C2'-C1'	2.81	106.53	103.13
1	A	579	CFZ	C3'-C2'-C1'	2.81	106.53	103.13
1	A	131	CFZ	C2'-C1'-N1	-2.81	109.91	114.20
1	B	418	CFZ	C2'-C1'-N1	-2.81	109.91	114.20
1	A	582	UFT	C2'-C3'-C4'	2.81	106.03	102.40
1	A	57	CFZ	C2'-C1'-N1	-2.81	109.91	114.20
1	A	600	CFZ	C2'-C1'-N1	-2.81	109.91	114.20
1	A	653	UFT	C3'-C2'-C1'	2.81	106.53	103.13
1	B	137	UFT	C2'-C1'-N1	-2.80	109.91	114.20
1	B	323	CFZ	C2'-C1'-N1	-2.80	109.92	114.20
1	B	407	CFZ	C3'-C2'-C1'	2.80	106.53	103.13
1	A	175	UFT	C2'-C3'-C4'	2.80	106.03	102.40
1	A	110	CFZ	C3'-C2'-C1'	2.80	106.52	103.13
1	B	206	CFZ	C3'-C2'-C1'	2.80	106.52	103.13
1	A	349	CFZ	C2'-C1'-N1	-2.80	109.92	114.20
1	A	215	UFT	O4-C4-C5	-2.80	120.23	125.16
1	B	535	UFT	O4-C4-C5	-2.80	120.23	125.16
1	A	669	UFT	C2'-C1'-N1	-2.80	109.92	114.20
1	A	604	CFZ	C2'-C1'-N1	-2.80	109.92	114.20
1	A	406	CFZ	C2'-C3'-C4'	2.80	106.02	102.40
1	B	309	UFT	C3'-C2'-C1'	2.80	106.52	103.13
1	B	499	UFT	C3'-C2'-C1'	2.80	106.52	103.13
1	B	124	CFZ	C2'-C1'-N1	-2.80	109.93	114.20
1	A	523	CFZ	C2'-C1'-N1	-2.80	109.93	114.20
1	B	153	UFT	C3'-C2'-C1'	2.79	106.51	103.13
1	A	657	CFZ	C2'-C3'-C4'	2.79	106.01	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	600	CFZ	C2'-C1'-N1	-2.79	109.94	114.20
1	B	88	UFT	C3'-C2'-C1'	2.79	106.51	103.13
1	A	659	UFT	C3'-C2'-C1'	2.79	106.51	103.13
1	A	76	CFZ	C2'-C3'-C4'	2.79	106.01	102.40
1	B	359	UFT	C3'-C2'-C1'	2.79	106.51	103.13
1	B	110	CFZ	C3'-C2'-C1'	2.79	106.50	103.13
1	A	554	UFT	C2'-C1'-N1	-2.79	109.94	114.20
1	A	359	UFT	O4-C4-C5	-2.79	120.26	125.16
1	B	92	UFT	C2'-C1'-N1	-2.78	109.94	114.20
1	B	369	CFZ	C2'-C3'-C4'	2.78	106.00	102.40
1	A	651	CFZ	C2'-C3'-C4'	2.78	106.00	102.40
1	A	407	CFZ	C2'-C1'-N1	-2.78	109.95	114.20
1	B	42	UFT	O4-C4-C5	-2.78	120.27	125.16
1	A	214	UFT	O4-C4-C5	-2.78	120.27	125.16
1	A	112	UFT	C3'-C2'-C1'	2.78	106.50	103.13
1	A	206	CFZ	C3'-C2'-C1'	2.78	106.50	103.13
1	B	365	UFT	C3'-C2'-C1'	2.78	106.50	103.13
1	A	524	UFT	O4-C4-C5	-2.78	120.27	125.16
1	B	304	CFZ	C2'-C1'-N1	-2.78	109.95	114.20
1	B	440	CFZ	C2'-C3'-C4'	2.78	106.00	102.40
1	A	153	UFT	C3'-C2'-C1'	2.78	106.50	103.13
1	A	14	UFT	O2-C2-N1	-2.78	119.09	122.79
1	B	296	UFT	C2'-C3'-C4'	2.78	106.00	102.40
1	A	387	CFZ	C2'-C3'-C4'	2.78	106.00	102.40
1	A	216	UFT	C1'-N1-C2	2.78	122.60	117.57
1	A	511	CFZ	C2'-C3'-C4'	2.78	106.00	102.40
1	A	662	UFT	C2'-C3'-C4'	2.78	106.00	102.40
1	B	523	CFZ	C2'-C3'-C4'	2.78	105.99	102.40
1	B	585	CFZ	C3'-C2'-C1'	2.78	106.50	103.13
1	A	462	CFZ	C2'-C1'-N1	-2.78	109.95	114.20
1	B	366	UFT	C2'-C3'-C4'	2.78	105.99	102.40
1	A	369	CFZ	C2'-C3'-C4'	2.78	105.99	102.40
1	B	423	UFT	C2'-C3'-C4'	2.78	105.99	102.40
1	B	32	UFT	C2'-C1'-N1	-2.78	109.96	114.20
1	A	19	UFT	C2'-C1'-N1	-2.78	109.96	114.20
1	B	493	UFT	C5-C4-N3	2.78	118.99	114.84
1	A	296	UFT	C2'-C3'-C4'	2.78	105.99	102.40
1	A	242	CFZ	C2'-C1'-N1	-2.77	109.96	114.20
1	A	302	UFT	C3'-C2'-C1'	2.77	106.49	103.13
1	B	407	CFZ	C2'-C1'-N1	-2.77	109.96	114.20
1	A	399	CFZ	C2'-C1'-N1	-2.77	109.96	114.20
1	A	204	UFT	C3'-C2'-C1'	2.77	106.48	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	CFZ	C2'-C3'-C4'	2.77	105.98	102.40
1	B	652	CFZ	C2'-C1'-N1	-2.77	109.97	114.20
1	B	139	CFZ	C2'-C3'-C4'	2.77	105.98	102.40
1	B	406	CFZ	C2'-C3'-C4'	2.77	105.98	102.40
1	A	363	CFZ	C2'-C1'-N1	-2.77	109.97	114.20
1	B	149	CFZ	C2'-C1'-N1	-2.77	109.97	114.20
1	B	21	CFZ	C3'-C2'-C1'	2.76	106.48	103.13
1	A	604	CFZ	C3'-C2'-C1'	2.76	106.48	103.13
1	B	579	CFZ	C2'-C1'-N1	-2.76	109.98	114.20
1	B	110	CFZ	C2'-C3'-C4'	2.76	105.97	102.40
1	A	156	CFZ	C2'-C3'-C4'	2.76	105.97	102.40
1	A	389	UFT	C2'-C1'-N1	-2.76	109.98	114.20
1	B	653	UFT	C2'-C1'-N1	-2.76	109.98	114.20
1	A	84	UFT	C3'-C2'-C1'	2.76	106.47	103.13
1	A	92	UFT	C2'-C1'-N1	-2.76	109.98	114.20
1	B	242	CFZ	C2'-C1'-N1	-2.76	109.99	114.20
1	A	55	UFT	C2'-C1'-N1	-2.76	109.99	114.20
1	B	651	CFZ	C2'-C3'-C4'	2.76	105.96	102.40
1	A	652	CFZ	C2'-C1'-N1	-2.76	109.99	114.20
1	A	285	CFZ	C2'-C1'-N1	-2.75	109.99	114.20
1	A	124	CFZ	C2'-C1'-N1	-2.75	110.00	114.20
1	A	198	CFZ	C2'-C1'-N1	-2.75	110.00	114.20
1	B	399	CFZ	C2'-C1'-N1	-2.75	110.00	114.20
1	B	279	CFZ	C2'-C1'-N1	-2.75	110.00	114.20
1	B	88	UFT	C2'-C1'-N1	-2.75	110.00	114.20
1	B	358	UFT	C3'-C2'-C1'	2.74	106.45	103.13
1	B	411	CFZ	C2'-C1'-N1	-2.74	110.01	114.20
1	B	696	UFT	C2'-C3'-C4'	2.74	105.94	102.40
1	A	232	CFZ	C2'-C1'-N1	-2.74	110.01	114.20
1	B	215	UFT	C2'-C1'-N1	-2.74	110.01	114.20
1	B	519	UFT	C2'-C1'-N1	-2.74	110.01	114.20
1	B	558	CFZ	C2'-C1'-N1	-2.74	110.02	114.20
1	A	653	UFT	C2'-C1'-N1	-2.74	110.02	114.20
1	A	524	UFT	C1'-N1-C2	2.74	122.52	117.57
1	A	684	UFT	C2'-C1'-N1	-2.73	110.02	114.20
1	B	477	CFZ	C2'-C1'-N1	-2.73	110.02	114.20
1	B	684	UFT	C2'-C1'-N1	-2.73	110.02	114.20
1	A	254	CFZ	C3'-C2'-C1'	2.73	106.44	103.13
1	A	523	CFZ	C2'-C3'-C4'	2.73	105.94	102.40
1	A	149	CFZ	C2'-C1'-N1	-2.73	110.03	114.20
1	B	216	UFT	C1'-N1-C2	2.73	122.52	117.57
1	A	8	UFT	C2'-C1'-N1	-2.73	110.03	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	CFZ	C3'-C2'-C1'	2.73	106.44	103.13
1	A	279	CFZ	C2'-C1'-N1	-2.73	110.03	114.20
1	A	491	CFZ	C2'-C3'-C4'	2.73	105.93	102.40
1	A	98	UFT	C3'-C2'-C1'	2.73	106.43	103.13
1	A	336	UFT	C2'-C3'-C4'	2.73	105.93	102.40
1	B	151	CFZ	C3'-C2'-C1'	2.73	106.43	103.13
1	B	76	CFZ	C2'-C1'-N1	-2.73	110.03	114.20
1	A	423	UFT	C2'-C3'-C4'	2.72	105.92	102.40
1	A	28	CFZ	C4'-O4'-C1'	-2.72	103.47	109.47
1	A	347	UFT	C3'-C2'-C1'	2.72	106.42	103.13
1	A	46	CFZ	C2'-C1'-N1	-2.72	110.04	114.20
1	A	423	UFT	C2'-C1'-N1	-2.72	110.04	114.20
1	B	34	CFZ	C2'-C3'-C4'	2.72	105.92	102.40
1	B	285	CFZ	C2'-C1'-N1	-2.72	110.04	114.20
1	A	179	UFT	C3'-C2'-C1'	2.72	106.42	103.13
1	A	110	CFZ	C2'-C3'-C4'	2.72	105.92	102.40
1	A	402	UFT	C3'-C2'-C1'	2.72	106.42	103.13
1	A	545	UFT	C3'-C2'-C1'	2.72	106.42	103.13
1	A	571	UFT	C3'-C2'-C1'	2.72	106.42	103.13
1	A	365	UFT	C2'-C1'-N1	-2.72	110.05	114.20
1	B	554	UFT	C2'-C1'-N1	-2.72	110.05	114.20
1	B	577	UFT	C2'-C1'-N1	-2.72	110.05	114.20
1	A	26	CFZ	C2'-C3'-C4'	2.71	105.91	102.40
1	A	700	CFZ	C2'-C3'-C4'	2.71	105.91	102.40
1	B	301	UFT	C3'-C2'-C1'	2.71	106.42	103.13
1	B	46	CFZ	C2'-C1'-N1	-2.71	110.05	114.20
1	B	691	CFZ	C2'-C1'-N1	-2.71	110.06	114.20
1	B	175	UFT	C3'-C2'-C1'	2.71	106.41	103.13
1	A	411	CFZ	C2'-C1'-N1	-2.71	110.06	114.20
1	B	208	UFT	C3'-C2'-C1'	2.71	106.41	103.13
1	A	696	UFT	C2'-C3'-C4'	2.71	105.90	102.40
1	A	245	UFT	C2'-C1'-N1	-2.71	110.06	114.20
1	A	369	CFZ	C2'-C1'-N1	-2.71	110.06	114.20
1	A	301	UFT	C3'-C2'-C1'	2.71	106.41	103.13
1	B	369	CFZ	C2'-C1'-N1	-2.70	110.07	114.20
1	B	534	UFT	C2'-C1'-N1	-2.70	110.07	114.20
1	A	19	UFT	C2'-C3'-C4'	2.70	105.90	102.40
1	A	208	UFT	C3'-C2'-C1'	2.70	106.40	103.13
1	A	421	UFT	C3'-C2'-C1'	2.70	106.40	103.13
1	A	405	CFZ	C2'-C1'-N1	-2.70	110.07	114.20
1	A	358	UFT	C3'-C2'-C1'	2.70	106.40	103.13
1	B	405	CFZ	C2'-C1'-N1	-2.70	110.07	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	CFZ	C2'-C1'-N1	-2.70	110.07	114.20
1	B	19	UFT	C3'-C2'-C1'	2.70	106.40	103.13
1	A	149	CFZ	C3'-C2'-C1'	2.70	106.40	103.13
1	A	42	UFT	C2'-C1'-N1	-2.70	110.07	114.20
1	A	350	UFT	C2'-C1'-N1	-2.70	110.07	114.20
1	A	34	CFZ	C2'-C1'-N1	-2.70	110.07	114.20
1	B	204	UFT	C3'-C2'-C1'	2.70	106.40	103.13
1	B	373	CFZ	C2'-C1'-N1	-2.70	110.08	114.20
1	B	504	UFT	C2'-C3'-C4'	2.69	105.89	102.40
1	B	175	UFT	C2'-C1'-N1	-2.69	110.08	114.20
1	A	373	CFZ	C2'-C1'-N1	-2.69	110.08	114.20
1	A	504	UFT	C2'-C3'-C4'	2.69	105.88	102.40
1	A	215	UFT	C2'-C1'-N1	-2.69	110.08	114.20
1	B	254	CFZ	C3'-C2'-C1'	2.69	106.39	103.13
1	A	667	CFZ	C2'-C1'-N1	-2.69	110.09	114.20
1	A	451	CFZ	C2'-C3'-C4'	2.69	105.88	102.40
1	A	322	UFT	C2'-C1'-N1	-2.69	110.09	114.20
1	A	477	CFZ	C2'-C1'-N1	-2.69	110.09	114.20
1	B	700	CFZ	C2'-C3'-C4'	2.69	105.88	102.40
1	B	131	CFZ	C3'-C2'-C1'	2.69	106.39	103.13
1	A	365	UFT	C3'-C2'-C1'	2.69	106.39	103.13
1	B	524	UFT	C2'-C1'-N1	-2.69	110.09	114.20
1	B	19	UFT	C2'-C1'-N1	-2.69	110.10	114.20
1	A	173	CFZ	C2'-C3'-C4'	2.68	105.87	102.40
1	A	691	CFZ	C2'-C1'-N1	-2.68	110.10	114.20
1	B	367	UFT	C2'-C1'-N1	-2.68	110.10	114.20
1	B	499	UFT	C2'-C3'-C4'	2.68	105.87	102.40
1	B	233	UFT	C3'-C2'-C1'	2.68	106.38	103.13
1	A	212	CFZ	C2'-C1'-N1	-2.68	110.10	114.20
1	A	49	CFZ	C3'-C2'-C1'	2.68	106.38	103.13
1	A	669	UFT	C3'-C2'-C1'	2.68	106.38	103.13
1	A	161	CFZ	C2'-C1'-N1	-2.68	110.10	114.20
1	A	106	UFT	C2'-C1'-N1	-2.68	110.11	114.20
1	B	411	CFZ	C3'-C2'-C1'	2.68	106.37	103.13
1	A	175	UFT	C3'-C2'-C1'	2.68	106.37	103.13
1	A	712	UFT	C2'-C1'-N1	-2.68	110.11	114.20
1	A	214	UFT	C2'-C1'-N1	-2.68	110.11	114.20
1	A	651	CFZ	C2'-C1'-N1	-2.68	110.11	114.20
1	B	690	UFT	C2'-C1'-N1	-2.68	110.11	114.20
1	B	198	CFZ	C2'-C1'-N1	-2.68	110.11	114.20
1	B	352	UFT	C2'-C3'-C4'	2.67	105.86	102.40
1	B	73	CFZ	C3'-C2'-C1'	2.67	106.37	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	CFZ	C3'-C2'-C1'	2.67	106.37	103.13
1	B	543	CFZ	C2'-C1'-N1	-2.67	110.12	114.20
1	A	690	UFT	C2'-C1'-N1	-2.67	110.12	114.20
1	A	545	UFT	C2'-C3'-C4'	2.67	105.85	102.40
1	A	666	UFT	C2'-C1'-N1	-2.67	110.12	114.20
1	B	402	UFT	C2'-C3'-C4'	2.67	105.85	102.40
1	A	245	UFT	C2'-C3'-C4'	2.67	105.85	102.40
1	B	206	CFZ	C2'-C1'-N1	-2.67	110.13	114.20
1	A	88	UFT	C2'-C1'-N1	-2.66	110.13	114.20
1	B	106	UFT	C2'-C1'-N1	-2.66	110.13	114.20
1	A	175	UFT	C2'-C1'-N1	-2.66	110.13	114.20
1	A	11	UFT	C2'-C1'-N1	-2.66	110.13	114.20
1	B	155	UFT	C2'-C1'-N1	-2.66	110.13	114.20
1	B	651	CFZ	C2'-C1'-N1	-2.66	110.13	114.20
1	B	441	CFZ	C2'-C3'-C4'	2.66	105.84	102.40
1	B	298	CFZ	C2'-C1'-N1	-2.66	110.13	114.20
1	B	679	CFZ	C2'-C3'-C4'	2.66	105.84	102.40
1	B	421	UFT	C3'-C2'-C1'	2.66	106.35	103.13
1	A	696	UFT	C2'-C1'-N1	-2.66	110.14	114.20
1	A	367	UFT	C2'-C1'-N1	-2.66	110.14	114.20
1	B	602	UFT	C3'-C2'-C1'	2.66	106.35	103.13
1	A	246	CFZ	C3'-C2'-C1'	2.66	106.35	103.13
1	A	558	CFZ	C2'-C1'-N1	-2.66	110.14	114.20
1	B	161	CFZ	C2'-C1'-N1	-2.66	110.14	114.20
1	B	493	UFT	O4-C4-C5	-2.66	120.49	125.16
1	A	151	CFZ	C3'-C2'-C1'	2.65	106.34	103.13
1	B	34	CFZ	C2'-C1'-N1	-2.65	110.14	114.20
1	A	309	UFT	C2'-C1'-N1	-2.65	110.14	114.20
1	A	593	UFT	C2'-C1'-N1	-2.65	110.14	114.20
1	B	198	CFZ	C2'-C3'-C4'	2.65	105.83	102.40
1	B	149	CFZ	C2'-C3'-C4'	2.65	105.83	102.40
1	A	666	UFT	C2'-C3'-C4'	2.65	105.83	102.40
1	A	80	UFT	C2'-C1'-N1	-2.65	110.15	114.20
1	A	206	CFZ	C2'-C1'-N1	-2.65	110.15	114.20
1	A	137	UFT	C3'-C2'-C1'	2.65	106.34	103.13
1	A	600	CFZ	C3'-C2'-C1'	2.65	106.34	103.13
1	A	411	CFZ	C3'-C2'-C1'	2.65	106.34	103.13
1	A	523	CFZ	C3'-C2'-C1'	2.65	106.34	103.13
1	B	600	CFZ	C3'-C2'-C1'	2.65	106.34	103.13
1	A	402	UFT	C2'-C3'-C4'	2.65	105.82	102.40
1	B	603	CFZ	C3'-C2'-C1'	2.65	106.33	103.13
1	A	72	CFZ	C2'-C1'-N1	-2.65	110.16	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	513	UFT	C2'-C1'-N1	-2.64	110.16	114.20
1	A	549	UFT	C2'-C3'-C4'	2.64	105.82	102.40
1	B	188	CFZ	C2'-C1'-N1	-2.64	110.16	114.20
1	A	592	CFZ	C2'-C3'-C4'	2.64	105.82	102.40
1	B	696	UFT	C2'-C1'-N1	-2.64	110.16	114.20
1	A	192	UFT	C2'-C3'-C4'	2.64	105.81	102.40
1	A	554	UFT	C2'-C3'-C4'	2.64	105.81	102.40
1	B	98	UFT	C3'-C2'-C1'	2.64	106.33	103.13
1	A	67	CFZ	C2'-C1'-N1	-2.64	110.17	114.20
1	A	491	CFZ	C2'-C1'-N1	-2.64	110.17	114.20
1	B	214	UFT	C2'-C1'-N1	-2.64	110.17	114.20
1	B	163	UFT	C3'-C2'-C1'	2.64	106.32	103.13
1	B	402	UFT	C3'-C2'-C1'	2.64	106.32	103.13
1	A	693	CFZ	C3'-C2'-C1'	2.64	106.32	103.13
1	A	704	CFZ	C2'-C1'-N1	-2.63	110.17	114.20
1	A	198	CFZ	C2'-C3'-C4'	2.63	105.81	102.40
1	A	217	UFT	C2'-C3'-C4'	2.63	105.81	102.40
1	B	667	CFZ	C2'-C1'-N1	-2.63	110.18	114.20
1	B	11	UFT	C2'-C3'-C4'	2.63	105.80	102.40
1	A	321	CFZ	C2'-C3'-C4'	2.63	105.80	102.40
1	B	545	UFT	C2'-C3'-C4'	2.63	105.80	102.40
1	B	351	CFZ	C2'-C1'-N1	-2.63	110.18	114.20
1	B	610	CFZ	C2'-C1'-N1	-2.63	110.18	114.20
1	B	72	CFZ	C3'-C2'-C1'	2.63	106.31	103.13
1	B	423	UFT	C2'-C1'-N1	-2.63	110.19	114.20
1	A	321	CFZ	C3'-C2'-C1'	2.63	106.31	103.13
1	A	325	CFZ	C2'-C1'-N1	-2.63	110.19	114.20
1	A	404	CFZ	C2'-C1'-N1	-2.63	110.19	114.20
1	A	88	UFT	C2'-C3'-C4'	2.63	105.80	102.40
1	B	404	CFZ	C2'-C1'-N1	-2.62	110.19	114.20
1	B	381	CFZ	C2'-C1'-N1	-2.62	110.19	114.20
1	A	76	CFZ	C3'-C2'-C1'	2.62	106.31	103.13
1	A	104	CFZ	C3'-C2'-C1'	2.62	106.31	103.13
1	B	137	UFT	C3'-C2'-C1'	2.62	106.31	103.13
1	A	188	CFZ	C2'-C3'-C4'	2.62	105.79	102.40
1	B	666	UFT	C2'-C1'-N1	-2.62	110.19	114.20
1	A	720	UFT	C2'-C1'-N1	-2.62	110.19	114.20
1	B	142	UFT	C2'-C1'-N1	-2.62	110.19	114.20
1	A	528	CFZ	C2'-C1'-N1	-2.62	110.19	114.20
1	B	155	UFT	C2'-C3'-C4'	2.62	105.79	102.40
1	A	358	UFT	C1'-N1-C2	2.62	122.31	117.57
1	B	647	CFZ	C2'-C1'-N1	-2.62	110.20	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	643	CFZ	C2'-C3'-C4'	2.62	105.79	102.40
1	B	389	UFT	C3'-C2'-C1'	2.62	106.30	103.13
1	B	545	UFT	C3'-C2'-C1'	2.62	106.30	103.13
1	B	693	CFZ	C3'-C2'-C1'	2.62	106.30	103.13
1	A	188	CFZ	C2'-C1'-N1	-2.62	110.20	114.20
1	B	358	UFT	O4-C4-C5	-2.62	120.56	125.16
1	B	528	CFZ	C2'-C1'-N1	-2.62	110.20	114.20
1	A	473	CFZ	C2'-C3'-C4'	2.62	105.78	102.40
1	B	440	CFZ	C2'-C1'-N1	-2.61	110.20	114.20
1	B	184	CFZ	C3'-C2'-C1'	2.61	106.29	103.13
1	A	534	UFT	C2'-C1'-N1	-2.61	110.21	114.20
1	A	639	CFZ	C2'-C1'-N1	-2.61	110.21	114.20
1	B	704	CFZ	C2'-C1'-N1	-2.61	110.21	114.20
1	B	545	UFT	C2'-C1'-N1	-2.61	110.21	114.20
1	B	423	UFT	C3'-C2'-C1'	2.61	106.29	103.13
1	A	155	UFT	C2'-C1'-N1	-2.61	110.21	114.20
1	B	309	UFT	C2'-C1'-N1	-2.61	110.21	114.20
1	A	142	UFT	C2'-C1'-N1	-2.61	110.21	114.20
1	A	543	CFZ	C2'-C1'-N1	-2.61	110.21	114.20
1	A	309	UFT	C2'-C3'-C4'	2.61	105.78	102.40
1	B	643	CFZ	C2'-C3'-C4'	2.61	105.78	102.40
1	B	687	UFT	C3'-C2'-C1'	2.61	106.29	103.13
1	B	80	UFT	C2'-C1'-N1	-2.61	110.22	114.20
1	A	229	UFT	C2'-C1'-N1	-2.61	110.22	114.20
1	A	28	CFZ	C3'-C2'-C1'	2.60	106.28	103.13
1	B	365	UFT	C2'-C1'-N1	-2.60	110.22	114.20
1	B	690	UFT	C3'-C2'-C1'	2.60	106.28	103.13
1	B	669	UFT	C2'-C3'-C4'	2.60	105.76	102.40
1	A	61	UFT	C2'-C1'-N1	-2.60	110.23	114.20
1	A	662	UFT	C2'-C1'-N1	-2.60	110.23	114.20
1	A	163	UFT	C3'-C2'-C1'	2.60	106.28	103.13
1	B	373	CFZ	C2'-C3'-C4'	2.60	105.76	102.40
1	A	545	UFT	C2'-C1'-N1	-2.60	110.23	114.20
1	B	92	UFT	C2'-C3'-C4'	2.60	105.76	102.40
1	A	704	CFZ	C2'-C3'-C4'	2.60	105.76	102.40
1	B	62	UFT	C2'-C1'-N1	-2.60	110.23	114.20
1	A	216	UFT	C2'-C3'-C4'	2.60	105.76	102.40
1	B	695	UFT	C3'-C2'-C1'	2.60	106.27	103.13
1	B	700	CFZ	C2'-C1'-N1	-2.59	110.23	114.20
1	B	309	UFT	C2'-C3'-C4'	2.59	105.76	102.40
1	B	542	UFT	C2'-C1'-N1	-2.59	110.23	114.20
1	B	592	CFZ	C2'-C3'-C4'	2.59	105.75	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	UFT	C3'-C2'-C1'	2.59	106.27	103.13
1	B	212	CFZ	C2'-C1'-N1	-2.59	110.24	114.20
1	B	511	CFZ	C2'-C3'-C4'	2.59	105.75	102.40
1	B	666	UFT	C2'-C3'-C4'	2.59	105.75	102.40
1	A	690	UFT	C3'-C2'-C1'	2.59	106.27	103.13
1	A	184	CFZ	C3'-C2'-C1'	2.59	106.26	103.13
1	A	398	UFT	C2'-C1'-N1	-2.59	110.25	114.20
1	B	602	UFT	C2'-C1'-N1	-2.59	110.25	114.20
1	A	59	UFT	C2'-C1'-N1	-2.59	110.25	114.20
1	B	55	UFT	C3'-C2'-C1'	2.59	106.26	103.13
1	A	373	CFZ	C2'-C3'-C4'	2.59	105.75	102.40
1	A	519	UFT	F2'-C2'-C3'	2.59	114.64	109.22
1	A	149	CFZ	C2'-C3'-C4'	2.59	105.74	102.40
1	B	188	CFZ	C2'-C3'-C4'	2.58	105.74	102.40
1	B	61	UFT	C2'-C1'-N1	-2.58	110.25	114.20
1	B	197	UFT	C2'-C1'-N1	-2.58	110.25	114.20
1	B	232	CFZ	C4'-O4'-C1'	-2.58	103.78	109.47
1	A	695	UFT	C3'-C2'-C1'	2.58	106.26	103.13
1	B	614	CFZ	C2'-C1'-N1	-2.58	110.25	114.20
1	B	639	CFZ	C2'-C1'-N1	-2.58	110.25	114.20
1	B	558	CFZ	C3'-C2'-C1'	2.58	106.25	103.13
1	A	34	CFZ	C2'-C3'-C4'	2.58	105.73	102.40
1	B	669	UFT	C2'-C1'-N1	-2.58	110.26	114.20
1	A	542	UFT	C2'-C3'-C4'	2.58	105.73	102.40
1	A	700	CFZ	C2'-C1'-N1	-2.58	110.26	114.20
1	B	104	CFZ	C3'-C2'-C1'	2.57	106.25	103.13
1	B	245	UFT	C3'-C2'-C1'	2.57	106.25	103.13
1	A	197	UFT	C2'-C1'-N1	-2.57	110.27	114.20
1	B	370	CFZ	C2'-C1'-N1	-2.57	110.27	114.20
1	A	558	CFZ	C3'-C2'-C1'	2.57	106.24	103.13
1	B	398	UFT	C2'-C3'-C4'	2.57	105.72	102.40
1	A	542	UFT	C2'-C1'-N1	-2.57	110.28	114.20
1	B	115	UFT	C2'-C1'-N1	-2.57	110.28	114.20
1	B	192	UFT	C2'-C3'-C4'	2.56	105.72	102.40
1	A	313	UFT	C3'-C2'-C1'	2.56	106.23	103.13
1	A	155	UFT	C2'-C3'-C4'	2.56	105.72	102.40
1	A	423	UFT	C3'-C2'-C1'	2.56	106.23	103.13
1	B	698	CFZ	C3'-C2'-C1'	2.56	106.23	103.13
1	A	296	UFT	C2'-C1'-N1	-2.56	110.28	114.20
1	A	434	UFT	C2'-C1'-N1	-2.56	110.28	114.20
1	B	704	CFZ	C2'-C3'-C4'	2.56	105.71	102.40
1	A	689	UFT	C2'-C1'-N1	-2.56	110.29	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	689	UFT	C2'-C1'-N1	-2.56	110.29	114.20
1	A	73	CFZ	C3'-C2'-C1'	2.56	106.23	103.13
1	A	614	CFZ	C3'-C2'-C1'	2.56	106.23	103.13
1	A	234	CFZ	C2'-C1'-N1	-2.56	110.29	114.20
1	A	19	UFT	C3'-C2'-C1'	2.56	106.22	103.13
1	B	635	UFT	C2'-C1'-N1	-2.56	110.29	114.20
1	A	687	UFT	C3'-C2'-C1'	2.55	106.22	103.13
1	B	190	UFT	C2'-C1'-N1	-2.55	110.30	114.20
1	B	322	UFT	C3'-C2'-C1'	2.55	106.22	103.13
1	B	481	UFT	C2'-C1'-N1	-2.55	110.30	114.20
1	B	504	UFT	C2'-C1'-N1	-2.55	110.30	114.20
1	A	635	UFT	C2'-C1'-N1	-2.55	110.31	114.20
1	B	266	UFT	C2'-C1'-N1	-2.55	110.31	114.20
1	A	402	UFT	C2'-C1'-N1	-2.55	110.31	114.20
1	B	662	UFT	C2'-C1'-N1	-2.55	110.31	114.20
1	A	266	UFT	C2'-C1'-N1	-2.54	110.31	114.20
1	B	653	UFT	C2'-C3'-C4'	2.54	105.69	102.40
1	A	587	CFZ	C3'-C2'-C1'	2.54	106.21	103.13
1	A	691	CFZ	C2'-C3'-C4'	2.54	105.69	102.40
1	B	548	CFZ	C2'-C1'-N1	-2.54	110.31	114.20
1	A	499	UFT	C2'-C3'-C4'	2.54	105.69	102.40
1	B	489	UFT	C3'-C2'-C1'	2.54	106.21	103.13
1	B	322	UFT	C2'-C1'-N1	-2.54	110.32	114.20
1	A	441	CFZ	C2'-C1'-N1	-2.54	110.32	114.20
1	A	519	UFT	C2'-C3'-C4'	2.54	105.69	102.40
1	A	387	CFZ	C3'-C2'-C1'	2.54	106.20	103.13
1	B	296	UFT	C2'-C1'-N1	-2.54	110.32	114.20
1	A	33	UFT	C3'-C2'-C1'	2.54	106.20	103.13
1	B	124	CFZ	C2'-C3'-C4'	2.54	105.68	102.40
1	B	383	CFZ	C2'-C3'-C4'	2.54	105.68	102.40
1	A	574	CFZ	C2'-C3'-C4'	2.54	105.68	102.40
1	A	115	UFT	C2'-C1'-N1	-2.54	110.33	114.20
1	A	76	CFZ	C2'-C1'-N1	-2.53	110.33	114.20
1	A	571	UFT	C2'-C1'-N1	-2.53	110.33	114.20
1	B	208	UFT	C2'-C3'-C4'	2.53	105.68	102.40
1	B	42	UFT	C1'-N1-C2	2.53	122.16	117.57
1	A	370	CFZ	C2'-C1'-N1	-2.53	110.33	114.20
1	A	607	UFT	C3'-C2'-C1'	2.53	106.20	103.13
1	A	504	UFT	C2'-C1'-N1	-2.53	110.33	114.20
1	B	201	CFZ	C2'-C1'-N1	-2.53	110.33	114.20
1	A	565	CFZ	C2'-C1'-N1	-2.53	110.33	114.20
1	A	124	CFZ	C2'-C3'-C4'	2.53	105.67	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	UFT	C2'-C1'-N1	-2.53	110.33	114.20
1	B	620	CFZ	C2'-C1'-N1	-2.53	110.33	114.20
1	B	551	CFZ	C3'-C2'-C1'	2.53	106.19	103.13
1	A	201	CFZ	C2'-C1'-N1	-2.53	110.33	114.20
1	A	585	CFZ	C2'-C3'-C4'	2.53	105.67	102.40
1	A	67	CFZ	C2'-C3'-C4'	2.53	105.67	102.40
1	A	698	CFZ	C3'-C2'-C1'	2.53	106.19	103.13
1	B	74	UFT	C2'-C1'-N1	-2.53	110.34	114.20
1	A	67	CFZ	C3'-C2'-C1'	2.53	106.19	103.13
1	A	355	CFZ	C2'-C1'-N1	-2.52	110.34	114.20
1	B	402	UFT	C2'-C1'-N1	-2.52	110.34	114.20
1	A	647	CFZ	C2'-C1'-N1	-2.52	110.34	114.20
1	A	164	CFZ	C2'-C3'-C4'	2.52	105.67	102.40
1	A	669	UFT	C2'-C3'-C4'	2.52	105.67	102.40
1	A	116	UFT	C2'-C1'-N1	-2.52	110.34	114.20
1	B	57	CFZ	C2'-C3'-C4'	2.52	105.66	102.40
1	A	215	UFT	C2'-C3'-C4'	2.52	105.66	102.40
1	B	398	UFT	C2'-C1'-N1	-2.52	110.34	114.20
1	B	88	UFT	C2'-C3'-C4'	2.52	105.66	102.40
1	A	607	UFT	C2'-C1'-N1	-2.52	110.35	114.20
1	B	378	CFZ	C2'-C3'-C4'	2.52	105.66	102.40
1	B	381	CFZ	C3'-C2'-C1'	2.52	106.18	103.13
1	B	691	CFZ	C2'-C3'-C4'	2.52	105.66	102.40
1	B	403	UFT	C2'-C1'-N1	-2.52	110.35	114.20
1	A	247	CFZ	C3'-C2'-C1'	2.52	106.18	103.13
1	B	21	CFZ	C2'-C1'-N1	-2.52	110.35	114.20
1	A	32	UFT	C2'-C1'-N1	-2.52	110.35	114.20
1	A	534	UFT	C2'-C3'-C4'	2.52	105.66	102.40
1	B	116	UFT	C2'-C1'-N1	-2.52	110.35	114.20
1	B	629	UFT	C2'-C1'-N1	-2.52	110.35	114.20
1	A	336	UFT	C2'-C1'-N1	-2.52	110.35	114.20
1	A	653	UFT	C2'-C3'-C4'	2.52	105.65	102.40
1	A	550	CFZ	C2'-C3'-C4'	2.52	105.65	102.40
1	B	33	UFT	C2'-C1'-N1	-2.51	110.36	114.20
1	B	434	UFT	C2'-C1'-N1	-2.51	110.36	114.20
1	B	120	CFZ	C2'-C1'-N1	-2.51	110.36	114.20
1	A	279	CFZ	C3'-C2'-C1'	2.51	106.17	103.13
1	A	120	CFZ	C2'-C1'-N1	-2.51	110.36	114.20
1	B	69	UFT	C2'-C1'-N1	-2.51	110.37	114.20
1	B	39	CFZ	O2-C2-N3	-2.51	118.25	122.33
1	A	421	UFT	C2'-C1'-N1	-2.50	110.37	114.20
1	A	325	CFZ	C2'-C3'-C4'	2.50	105.64	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	UFT	C3'-C2'-C1'	2.50	106.16	103.13
1	A	313	UFT	C2'-C3'-C4'	2.50	105.64	102.40
1	B	316	CFZ	C3'-C2'-C1'	2.50	106.16	103.13
1	A	378	CFZ	C2'-C3'-C4'	2.50	105.64	102.40
1	B	217	UFT	C2'-C3'-C4'	2.50	105.63	102.40
1	A	603	CFZ	C3'-C2'-C1'	2.50	106.16	103.13
1	B	614	CFZ	C3'-C2'-C1'	2.50	106.16	103.13
1	B	542	UFT	C2'-C3'-C4'	2.50	105.63	102.40
1	A	169	UFT	C2'-C1'-N1	-2.50	110.38	114.20
1	B	94	UFT	C2'-C1'-N1	-2.50	110.39	114.20
1	A	609	UFT	C2'-C1'-N1	-2.50	110.39	114.20
1	B	84	UFT	C2'-C1'-N1	-2.49	110.39	114.20
1	B	234	CFZ	C2'-C1'-N1	-2.49	110.39	114.20
1	B	568	CFZ	C2'-C3'-C4'	2.49	105.63	102.40
1	B	43	UFT	O4'-C1'-N1	2.49	114.06	108.36
1	B	614	CFZ	C2'-C3'-C4'	2.49	105.62	102.40
1	B	676	UFT	C1'-N1-C2	2.49	122.08	117.57
1	B	246	CFZ	C2'-C1'-N1	-2.49	110.40	114.20
1	B	491	CFZ	C2'-C1'-N1	-2.49	110.40	114.20
1	A	494	CFZ	C2'-C1'-N1	-2.49	110.40	114.20
1	B	549	UFT	C2'-C1'-N1	-2.49	110.40	114.20
1	B	551	CFZ	C2'-C1'-N1	-2.49	110.40	114.20
1	B	76	CFZ	C2'-C3'-C4'	2.49	105.62	102.40
1	A	528	CFZ	C3'-C2'-C1'	2.49	106.14	103.13
1	B	57	CFZ	C2'-C1'-N1	-2.49	110.40	114.20
1	B	636	UFT	C2'-C1'-N1	-2.48	110.40	114.20
1	A	112	UFT	C2'-C1'-N1	-2.48	110.40	114.20
1	A	481	UFT	C2'-C1'-N1	-2.48	110.41	114.20
1	B	351	CFZ	C2'-C3'-C4'	2.48	105.61	102.40
1	A	548	CFZ	C2'-C1'-N1	-2.48	110.41	114.20
1	A	682	CFZ	C3'-C2'-C1'	2.48	106.14	103.13
1	A	33	UFT	C2'-C1'-N1	-2.48	110.41	114.20
1	A	620	CFZ	C2'-C1'-N1	-2.48	110.41	114.20
1	A	629	UFT	C2'-C1'-N1	-2.48	110.41	114.20
1	B	249	CFZ	C3'-C2'-C1'	2.48	106.13	103.13
1	A	421	UFT	C2'-C3'-C4'	2.48	105.61	102.40
1	A	26	CFZ	C2'-C1'-N1	-2.48	110.41	114.20
1	B	682	CFZ	C3'-C2'-C1'	2.47	106.13	103.13
1	A	398	UFT	C2'-C3'-C4'	2.47	105.60	102.40
1	B	421	UFT	C2'-C3'-C4'	2.47	105.60	102.40
1	A	498	CFZ	C2'-C3'-C4'	2.47	105.60	102.40
1	B	719	UFT	C2'-C3'-C4'	2.47	105.60	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	CFZ	C2'-C1'-N1	-2.47	110.42	114.20
1	B	701	UFT	C2'-C1'-N1	-2.47	110.42	114.20
1	B	245	UFT	C2'-C1'-N1	-2.47	110.42	114.20
1	B	609	UFT	C2'-C1'-N1	-2.47	110.42	114.20
1	A	568	CFZ	C2'-C3'-C4'	2.47	105.59	102.40
1	A	39	CFZ	O2-C2-N3	-2.47	118.31	122.33
1	A	499	UFT	C2'-C1'-N1	-2.47	110.43	114.20
1	A	98	UFT	C2'-C3'-C4'	2.47	105.59	102.40
1	A	528	CFZ	C2'-C3'-C4'	2.47	105.59	102.40
1	A	63	CFZ	C2'-C1'-N1	-2.47	110.43	114.20
1	B	169	UFT	C2'-C1'-N1	-2.47	110.43	114.20
1	A	403	UFT	C2'-C1'-N1	-2.47	110.43	114.20
1	B	421	UFT	C2'-C1'-N1	-2.47	110.43	114.20
1	A	676	UFT	C1'-N1-C2	2.47	122.04	117.57
1	B	298	CFZ	C2'-C3'-C4'	2.47	105.59	102.40
1	B	558	CFZ	C2'-C3'-C4'	2.47	105.59	102.40
1	B	112	UFT	C2'-C1'-N1	-2.47	110.43	114.20
1	B	25	CFZ	O4'-C1'-C2'	2.46	108.33	105.79
1	B	585	CFZ	C2'-C3'-C4'	2.46	105.58	102.40
1	A	581	UFT	C2'-C1'-N1	-2.46	110.44	114.20
1	A	441	CFZ	C3'-C2'-C1'	2.46	106.11	103.13
1	B	530	UFT	C2'-C1'-N1	-2.46	110.44	114.20
1	A	701	UFT	C2'-C1'-N1	-2.46	110.44	114.20
1	B	215	UFT	C2'-C3'-C4'	2.46	105.58	102.40
1	B	117	CFZ	C2'-C1'-N1	-2.46	110.44	114.20
1	A	192	UFT	C2'-C1'-N1	-2.46	110.44	114.20
1	A	43	UFT	O4'-C1'-N1	2.46	113.98	108.36
1	A	190	UFT	C2'-C1'-N1	-2.46	110.45	114.20
1	B	418	CFZ	C2'-C3'-C4'	2.46	105.58	102.40
1	B	57	CFZ	C3'-C2'-C1'	2.46	106.10	103.13
1	B	279	CFZ	C3'-C2'-C1'	2.46	106.10	103.13
1	A	208	UFT	C2'-C3'-C4'	2.45	105.58	102.40
1	A	209	CFZ	C3'-C2'-C1'	2.45	106.10	103.13
1	B	209	CFZ	C3'-C2'-C1'	2.45	106.10	103.13
1	B	524	UFT	C3'-C2'-C1'	2.45	106.10	103.13
1	B	160	UFT	C2'-C1'-N1	-2.45	110.45	114.20
1	A	55	UFT	C3'-C2'-C1'	2.45	106.10	103.13
1	A	455	CFZ	C2'-C1'-N1	-2.45	110.45	114.20
1	B	151	CFZ	C2'-C1'-N1	-2.45	110.45	114.20
1	B	581	UFT	C2'-C1'-N1	-2.45	110.46	114.20
1	B	153	UFT	C2'-C1'-N1	-2.45	110.46	114.20
1	B	336	UFT	C2'-C1'-N1	-2.45	110.46	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	UFT	C2'-C1'-N1	-2.45	110.46	114.20
1	B	534	UFT	C2'-C3'-C4'	2.45	105.56	102.40
1	A	411	CFZ	C2'-C3'-C4'	2.44	105.56	102.40
1	A	59	UFT	C2'-C3'-C4'	2.44	105.56	102.40
1	B	474	CFZ	C2'-C3'-C4'	2.44	105.56	102.40
1	A	11	UFT	C3'-C2'-C1'	2.44	106.09	103.13
1	A	322	UFT	C3'-C2'-C1'	2.44	106.09	103.13
1	B	63	CFZ	C2'-C1'-N1	-2.44	110.47	114.20
1	B	325	CFZ	C2'-C1'-N1	-2.44	110.47	114.20
1	A	418	CFZ	C2'-C3'-C4'	2.44	105.56	102.40
1	A	637	CFZ	C2'-C1'-N1	-2.44	110.47	114.20
1	A	62	UFT	C2'-C1'-N1	-2.44	110.47	114.20
1	A	602	UFT	C3'-C2'-C1'	2.44	106.08	103.13
1	A	298	CFZ	C2'-C3'-C4'	2.44	105.55	102.40
1	A	636	UFT	C2'-C1'-N1	-2.44	110.48	114.20
1	A	426	CFZ	C2'-C3'-C4'	2.43	105.55	102.40
1	A	57	CFZ	C3'-C2'-C1'	2.43	106.08	103.13
1	B	565	CFZ	C2'-C1'-N1	-2.43	110.48	114.20
1	A	556	CFZ	C3'-C2'-C1'	2.43	106.07	103.13
1	A	110	CFZ	C2'-C1'-N1	-2.43	110.48	114.20
1	A	160	UFT	C2'-C1'-N1	-2.43	110.48	114.20
1	B	28	CFZ	C2'-C3'-C4'	-2.43	99.26	102.40
1	A	75	CFZ	O4'-C1'-C2'	2.43	108.29	105.79
1	B	355	CFZ	C3'-C2'-C1'	2.43	106.07	103.13
1	A	316	CFZ	C3'-C2'-C1'	2.43	106.07	103.13
1	B	143	UFT	C2'-C1'-N1	-2.43	110.49	114.20
1	B	664	CFZ	C2'-C1'-N1	-2.43	110.49	114.20
1	A	84	UFT	C2'-C1'-N1	-2.42	110.49	114.20
1	A	349	CFZ	C3'-C2'-C1'	2.42	106.06	103.13
1	B	157	CFZ	C3'-C2'-C1'	2.42	106.06	103.13
1	A	21	CFZ	C2'-C1'-N1	-2.42	110.50	114.20
1	A	583	CFZ	C2'-C1'-N1	-2.42	110.50	114.20
1	B	219	CFZ	C3'-C2'-C1'	2.42	106.06	103.13
1	B	42	UFT	C3'-C2'-C1'	2.42	106.06	103.13
1	A	170	UFT	C2'-C1'-N1	-2.42	110.51	114.20
1	B	411	CFZ	C2'-C3'-C4'	2.42	105.53	102.40
1	A	474	CFZ	C2'-C3'-C4'	2.42	105.53	102.40
1	B	528	CFZ	C2'-C3'-C4'	2.42	105.53	102.40
1	A	117	CFZ	C2'-C1'-N1	-2.42	110.51	114.20
1	A	80	UFT	C3'-C2'-C1'	2.41	106.05	103.13
1	B	76	CFZ	C3'-C2'-C1'	2.41	106.05	103.13
1	B	637	CFZ	C2'-C1'-N1	-2.41	110.52	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	CFZ	C2'-C3'-C4'	2.41	105.52	102.40
1	B	71	UFT	C2'-C1'-N1	-2.41	110.52	114.20
1	B	98	UFT	C2'-C3'-C4'	2.40	105.51	102.40
1	A	574	CFZ	C3'-C2'-C1'	2.40	106.04	103.13
1	B	425	CFZ	C2'-C3'-C4'	2.40	105.51	102.40
1	A	249	CFZ	C3'-C2'-C1'	2.40	106.04	103.13
1	B	582	UFT	C3'-C2'-C1'	2.40	106.04	103.13
1	A	519	UFT	C2'-C1'-N1	-2.40	110.53	114.20
1	A	664	CFZ	C2'-C1'-N1	-2.40	110.53	114.20
1	A	325	CFZ	C3'-C2'-C1'	2.40	106.04	103.13
1	B	214	UFT	C2'-C3'-C4'	2.40	105.50	102.40
1	B	568	CFZ	C3'-C2'-C1'	2.40	106.03	103.13
1	A	568	CFZ	C3'-C2'-C1'	2.40	106.03	103.13
1	A	49	CFZ	C2'-C3'-C4'	2.39	105.50	102.40
1	A	92	UFT	C2'-C3'-C4'	2.39	105.50	102.40
1	A	530	UFT	C3'-C2'-C1'	2.39	106.03	103.13
1	B	110	CFZ	C2'-C1'-N1	-2.39	110.54	114.20
1	B	202	UFT	C2'-C1'-N1	-2.39	110.54	114.20
1	B	407	CFZ	C2'-C3'-C4'	2.39	105.49	102.40
1	A	72	CFZ	C2'-C3'-C4'	2.39	105.49	102.40
1	A	513	UFT	C3'-C2'-C1'	2.39	106.03	103.13
1	B	90	CFZ	C2'-C1'-N1	-2.39	110.55	114.20
1	B	44	UFT	C3'-C2'-C1'	2.39	106.02	103.13
1	B	583	CFZ	C2'-C1'-N1	-2.39	110.55	114.20
1	A	153	UFT	C2'-C1'-N1	-2.39	110.55	114.20
1	A	462	CFZ	C2'-C3'-C4'	2.39	105.49	102.40
1	B	528	CFZ	C3'-C2'-C1'	2.39	106.02	103.13
1	A	469	CFZ	C2'-C1'-N1	-2.38	110.56	114.20
1	B	625	CFZ	C2'-C1'-N1	-2.38	110.56	114.20
1	A	425	CFZ	C2'-C3'-C4'	2.38	105.48	102.40
1	B	101	UFT	C2'-C1'-N1	-2.38	110.57	114.20
1	A	10	CFZ	C3'-C2'-C1'	2.38	106.01	103.13
1	B	351	CFZ	C3'-C2'-C1'	2.38	106.01	103.13
1	A	582	UFT	C3'-C2'-C1'	2.38	106.01	103.13
1	A	97	UFT	C2'-C3'-C4'	2.37	105.47	102.40
1	A	625	CFZ	C2'-C1'-N1	-2.37	110.57	114.20
1	A	506	CFZ	C2'-C1'-N1	-2.37	110.58	114.20
1	A	559	UFT	C2'-C1'-N1	-2.37	110.58	114.20
1	B	170	UFT	C2'-C1'-N1	-2.37	110.58	114.20
1	A	500	UFT	C2'-C1'-N1	-2.37	110.58	114.20
1	B	431	UFT	C2'-C1'-N1	-2.37	110.58	114.20
1	A	659	UFT	C1'-N1-C2	2.37	121.86	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	CFZ	C3'-C2'-C1'	2.37	105.99	103.13
1	A	46	CFZ	C2'-C3'-C4'	2.36	105.46	102.40
1	B	344	UFT	C2'-C3'-C4'	2.36	105.46	102.40
1	B	11	UFT	C2'-C1'-N1	-2.36	110.59	114.20
1	B	587	CFZ	C3'-C2'-C1'	2.36	105.99	103.13
1	A	407	CFZ	C2'-C3'-C4'	2.36	105.45	102.40
1	B	669	UFT	C3'-C2'-C1'	2.36	105.99	103.13
1	B	659	UFT	C1'-N1-C2	2.36	121.84	117.57
1	B	593	UFT	C2'-C3'-C4'	2.36	105.45	102.40
1	A	441	CFZ	C2'-C3'-C4'	2.36	105.45	102.40
1	B	80	UFT	C3'-C2'-C1'	2.36	105.98	103.13
1	A	444	CFZ	C2'-C1'-N1	-2.36	110.60	114.20
1	B	489	UFT	C2'-C3'-C4'	2.35	105.45	102.40
1	B	79	CFZ	C2'-C1'-N1	-2.35	110.60	114.20
1	B	608	UFT	C2'-C1'-N1	-2.35	110.61	114.20
1	B	46	CFZ	C2'-C3'-C4'	2.35	105.44	102.40
1	B	355	CFZ	C2'-C1'-N1	-2.35	110.61	114.20
1	A	425	CFZ	C2'-C1'-N1	-2.35	110.61	114.20
1	B	469	CFZ	C2'-C1'-N1	-2.35	110.61	114.20
1	A	157	CFZ	C3'-C2'-C1'	2.35	105.98	103.13
1	A	350	UFT	C3'-C2'-C1'	2.35	105.98	103.13
1	B	489	UFT	C2'-C1'-N1	-2.35	110.61	114.20
1	A	332	CFZ	C2'-C1'-N1	-2.35	110.61	114.20
1	A	406	CFZ	C2'-C1'-N1	-2.34	110.62	114.20
1	B	524	UFT	C2'-C3'-C4'	2.34	105.43	102.40
1	B	506	CFZ	C2'-C1'-N1	-2.34	110.62	114.20
1	A	232	CFZ	C2'-C3'-C4'	2.34	105.43	102.40
1	A	89	UFT	C2'-C1'-N1	-2.34	110.62	114.20
1	A	534	UFT	C3'-C2'-C1'	2.34	105.96	103.13
1	B	406	CFZ	C2'-C1'-N1	-2.34	110.63	114.20
1	B	232	CFZ	C2'-C1'-N1	-2.34	110.63	114.20
1	A	608	UFT	C2'-C1'-N1	-2.34	110.63	114.20
1	A	607	UFT	C2'-C3'-C4'	2.34	105.42	102.40
1	A	210	CFZ	C4'-O4'-C1'	-2.34	104.32	109.47
1	B	196	UFT	C1'-N1-C2	2.33	121.80	117.57
1	B	500	UFT	C2'-C1'-N1	-2.33	110.63	114.20
1	B	188	CFZ	C3'-C2'-C1'	2.33	105.96	103.13
1	B	210	CFZ	C4'-O4'-C1'	-2.33	104.33	109.47
1	A	188	CFZ	C3'-C2'-C1'	2.33	105.95	103.13
1	B	574	CFZ	C3'-C2'-C1'	2.33	105.95	103.13
1	B	607	UFT	C2'-C1'-N1	-2.33	110.64	114.20
1	A	196	UFT	C1'-N1-C2	2.33	121.79	117.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	CFZ	C2'-C1'-N1	-2.33	110.64	114.20
1	B	604	CFZ	C2'-C3'-C4'	2.33	105.41	102.40
1	B	633	UFT	O2-C2-N1	-2.33	119.69	122.79
1	A	42	UFT	C3'-C2'-C1'	2.33	105.95	103.13
1	B	498	CFZ	C2'-C3'-C4'	2.33	105.41	102.40
1	A	21	CFZ	C2'-C3'-C4'	2.33	105.41	102.40
1	A	359	UFT	C2'-C3'-C4'	2.33	105.41	102.40
1	B	687	UFT	C2'-C3'-C4'	2.33	105.41	102.40
1	B	283	UFT	O2-C2-N1	-2.33	119.69	122.79
1	A	663	UFT	C2'-C1'-N1	-2.32	110.65	114.20
1	A	84	UFT	C2'-C3'-C4'	2.32	105.40	102.40
1	A	302	UFT	C2'-C1'-N1	-2.32	110.65	114.20
1	A	687	UFT	C2'-C3'-C4'	2.32	105.40	102.40
1	B	332	CFZ	C2'-C1'-N1	-2.32	110.65	114.20
1	A	629	UFT	C3'-C2'-C1'	2.32	105.94	103.13
1	B	446	CFZ	O4'-C1'-C2'	2.32	108.18	105.79
1	A	413	UFT	C2'-C1'-N1	-2.32	110.65	114.20
1	B	144	CFZ	C2'-C1'-N1	-2.32	110.66	114.20
1	A	283	UFT	O2-C2-N1	-2.32	119.71	122.79
1	B	629	UFT	C3'-C2'-C1'	2.32	105.94	103.13
1	B	652	CFZ	C2'-C3'-C4'	2.32	105.39	102.40
1	A	509	UFT	C2'-C1'-N1	-2.31	110.66	114.20
1	A	389	UFT	C3'-C2'-C1'	2.31	105.93	103.13
1	A	652	CFZ	C2'-C3'-C4'	2.31	105.39	102.40
1	A	618	UFT	C2'-C1'-N1	-2.31	110.67	114.20
1	B	354	CFZ	C2'-C1'-N1	-2.31	110.67	114.20
1	B	663	UFT	C2'-C1'-N1	-2.31	110.67	114.20
1	B	302	UFT	C2'-C1'-N1	-2.31	110.67	114.20
1	B	251	UFT	C2'-C3'-C4'	2.31	105.39	102.40
1	A	477	CFZ	C3'-C2'-C1'	2.31	105.92	103.13
1	B	179	UFT	C2'-C3'-C4'	2.31	105.39	102.40
1	B	14	UFT	O2-C2-N1	-2.31	119.72	122.79
1	A	137	UFT	C2'-C3'-C4'	2.31	105.38	102.40
1	A	610	CFZ	C2'-C1'-N1	-2.31	110.68	114.20
1	B	593	UFT	C2'-C1'-N1	-2.30	110.68	114.20
1	A	44	UFT	C3'-C2'-C1'	2.30	105.92	103.13
1	A	144	CFZ	C2'-C1'-N1	-2.30	110.69	114.20
1	A	633	UFT	O2-C2-N1	-2.30	119.73	122.79
1	A	156	CFZ	O2-C2-N3	-2.30	118.59	122.33
1	B	55	UFT	C2'-C3'-C4'	2.30	105.37	102.40
1	A	219	CFZ	C2'-C3'-C4'	2.30	105.37	102.40
1	A	19	UFT	O2-C2-N1	-2.30	119.73	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	UFT	C3'-C2'-C1'	2.29	105.91	103.13
1	A	455	CFZ	C2'-C3'-C4'	2.29	105.37	102.40
1	B	509	UFT	C2'-C1'-N1	-2.29	110.69	114.20
1	A	712	UFT	C2'-C3'-C4'	2.29	105.37	102.40
1	B	602	UFT	C2'-C3'-C4'	2.29	105.36	102.40
1	A	179	UFT	C2'-C3'-C4'	2.29	105.36	102.40
1	B	97	UFT	C2'-C1'-N1	-2.29	110.70	114.20
1	A	329	UFT	C2'-C3'-C4'	2.29	105.36	102.40
1	B	559	UFT	C2'-C1'-N1	-2.29	110.70	114.20
1	A	103	CFZ	C2'-C1'-N1	-2.29	110.71	114.20
1	B	216	UFT	C2'-C3'-C4'	2.28	105.36	102.40
1	B	304	CFZ	C3'-C2'-C1'	2.28	105.89	103.13
1	B	606	UFT	O2-C2-N1	-2.28	119.75	122.79
1	A	164	CFZ	C2'-C1'-N1	-2.28	110.71	114.20
1	A	477	CFZ	C2'-C3'-C4'	2.28	105.35	102.40
1	A	690	UFT	C2'-C3'-C4'	2.28	105.35	102.40
1	B	477	CFZ	C2'-C3'-C4'	2.28	105.34	102.40
1	A	446	CFZ	O4'-C1'-C2'	2.28	108.14	105.79
1	B	441	CFZ	O2-C2-N3	-2.28	118.63	122.33
1	A	74	UFT	C2'-C1'-N1	-2.27	110.73	114.20
1	B	366	UFT	C2'-C1'-N1	-2.27	110.73	114.20
1	A	233	UFT	C2'-C3'-C4'	2.27	105.34	102.40
1	A	126	UFT	C2'-C1'-N1	-2.27	110.73	114.20
1	A	219	CFZ	C3'-C2'-C1'	2.27	105.88	103.13
1	B	43	UFT	C2'-C1'-N1	-2.27	110.73	114.20
1	B	425	CFZ	C2'-C1'-N1	-2.27	110.74	114.20
1	B	49	CFZ	O2-C2-N3	-2.26	118.65	122.33
1	B	241	CFZ	O4'-C1'-C2'	2.26	108.12	105.79
1	A	530	UFT	C2'-C3'-C4'	2.26	105.33	102.40
1	B	49	CFZ	C3'-C2'-C1'	2.26	105.87	103.13
1	B	171	CFZ	C2'-C1'-N1	-2.26	110.74	114.20
1	B	89	UFT	C2'-C1'-N1	-2.26	110.75	114.20
1	A	334	UFT	C2'-C1'-N1	-2.26	110.75	114.20
1	A	657	CFZ	F2'-C2'-C3'	2.26	113.95	109.22
1	B	80	UFT	C2'-C3'-C4'	2.26	105.32	102.40
1	A	384	CFZ	C2'-C1'-N1	-2.26	110.75	114.20
1	B	439	CFZ	O4'-C1'-C2'	2.26	108.11	105.79
1	A	298	CFZ	C3'-C2'-C1'	2.26	105.86	103.13
1	B	323	CFZ	C2'-C3'-C4'	2.25	105.32	102.40
1	B	59	UFT	C2'-C1'-N1	-2.25	110.76	114.20
1	B	137	UFT	C2'-C3'-C4'	2.25	105.31	102.40
1	A	576	CFZ	O4'-C1'-C2'	2.25	108.11	105.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	CFZ	C2'-C1'-N1	-2.25	110.76	114.20
1	B	438	CFZ	C2'-C1'-N1	-2.25	110.76	114.20
1	A	43	UFT	C2'-C1'-N1	-2.25	110.76	114.20
1	A	241	CFZ	O4'-C1'-C2'	2.25	108.11	105.79
1	B	293	UFT	C2'-C3'-C4'	2.25	105.31	102.40
1	B	126	UFT	C2'-C1'-N1	-2.25	110.77	114.20
1	B	404	CFZ	C2'-C3'-C4'	2.25	105.31	102.40
1	A	55	UFT	C2'-C3'-C4'	2.25	105.30	102.40
1	A	351	CFZ	C2'-C3'-C4'	2.25	105.30	102.40
1	A	322	UFT	C1'-N1-C2	2.24	121.63	117.57
1	A	558	CFZ	C2'-C3'-C4'	2.24	105.30	102.40
1	A	293	UFT	C2'-C3'-C4'	2.24	105.30	102.40
1	B	708	UFT	O2-C2-N1	-2.24	119.81	122.79
1	B	219	CFZ	C2'-C3'-C4'	2.24	105.30	102.40
1	A	512	CFZ	C3'-C2'-C1'	2.24	105.84	103.13
1	B	579	CFZ	C2'-C3'-C4'	2.24	105.30	102.40
1	A	600	CFZ	C2'-C3'-C4'	2.24	105.30	102.40
1	A	86	UFT	C2'-C3'-C4'	2.24	105.30	102.40
1	A	363	CFZ	C3'-C2'-C1'	2.24	105.84	103.13
1	A	438	CFZ	C2'-C1'-N1	-2.23	110.79	114.20
1	B	334	UFT	C2'-C1'-N1	-2.23	110.79	114.20
1	A	387	CFZ	C2'-C1'-N1	-2.23	110.79	114.20
1	B	477	CFZ	C3'-C2'-C1'	2.23	105.83	103.13
1	A	579	CFZ	C2'-C3'-C4'	2.23	105.29	102.40
1	B	120	CFZ	O2-C2-N3	-2.23	118.70	122.33
1	B	86	UFT	C3'-C2'-C1'	2.23	105.83	103.13
1	A	302	UFT	C1'-N1-C2	2.23	121.61	117.57
1	A	417	CFZ	O4'-C1'-C2'	2.23	108.09	105.79
1	A	404	CFZ	C2'-C3'-C4'	2.23	105.28	102.40
1	B	571	UFT	C2'-C1'-N1	-2.23	110.80	114.20
1	A	251	UFT	C2'-C3'-C4'	2.23	105.28	102.40
1	A	366	UFT	C2'-C1'-N1	-2.23	110.80	114.20
1	A	254	CFZ	C2'-C3'-C4'	2.22	105.28	102.40
1	B	492	CFZ	C2'-C3'-C4'	2.22	105.28	102.40
1	B	600	CFZ	C2'-C3'-C4'	2.22	105.28	102.40
1	B	302	UFT	C1'-N1-C2	2.22	121.60	117.57
1	A	232	CFZ	C4'-O4'-C1'	-2.22	104.57	109.47
1	A	11	UFT	C2'-C3'-C4'	2.22	105.28	102.40
1	A	439	CFZ	O2-C2-N3	-2.22	118.72	122.33
1	B	112	UFT	C2'-C3'-C4'	2.22	105.27	102.40
1	B	44	UFT	C2'-C3'-C4'	2.22	105.27	102.40
1	B	618	UFT	C2'-C1'-N1	-2.22	110.81	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	UFT	O2-C2-N1	-2.22	119.84	122.79
1	A	10	CFZ	O2-C2-N3	-2.21	118.73	122.33
1	B	534	UFT	C3'-C2'-C1'	2.21	105.81	103.13
1	A	604	CFZ	C2'-C3'-C4'	2.21	105.26	102.40
1	A	165	CFZ	C3'-C2'-C1'	2.21	105.81	103.13
1	A	647	CFZ	C2'-C3'-C4'	2.21	105.25	102.40
1	B	298	CFZ	C3'-C2'-C1'	2.20	105.80	103.13
1	B	431	UFT	O2-C2-N1	-2.20	119.86	122.79
1	B	163	UFT	C2'-C3'-C4'	2.20	105.25	102.40
1	A	352	UFT	C2'-C1'-N1	-2.20	110.83	114.20
1	B	49	CFZ	C2'-C1'-N1	-2.20	110.84	114.20
1	A	282	CFZ	O4'-C1'-C2'	2.20	108.06	105.79
1	B	491	CFZ	C3'-C2'-C1'	2.20	105.79	103.13
1	A	90	CFZ	C2'-C1'-N1	-2.20	110.84	114.20
1	A	708	UFT	O2-C2-N1	-2.20	119.86	122.79
1	B	304	CFZ	C2'-C3'-C4'	2.20	105.24	102.40
1	A	431	UFT	C2'-C1'-N1	-2.20	110.84	114.20
1	A	120	CFZ	O2-C2-N3	-2.20	118.76	122.33
1	B	493	UFT	O2-C2-N3	-2.20	117.41	121.50
1	A	192	UFT	C3'-C2'-C1'	2.20	105.79	103.13
1	A	163	UFT	C2'-C3'-C4'	2.20	105.24	102.40
1	B	353	CFZ	C2'-C1'-N1	-2.20	110.84	114.20
1	A	633	UFT	C3'-C2'-C1'	2.19	105.79	103.13
1	B	329	UFT	C2'-C3'-C4'	2.19	105.24	102.40
1	B	26	CFZ	C4'-O4'-C1'	-2.19	104.64	109.47
1	B	690	UFT	C2'-C3'-C4'	2.19	105.23	102.40
1	A	115	UFT	O2-C2-N1	-2.19	119.88	122.79
1	A	69	UFT	C2'-C1'-N1	-2.19	110.85	114.20
1	B	719	UFT	C2'-C1'-N1	-2.19	110.85	114.20
1	B	621	UFT	C2'-C1'-N1	-2.19	110.86	114.20
1	B	92	UFT	C3'-C2'-C1'	2.19	105.78	103.13
1	A	354	CFZ	F2'-C2'-C3'	2.19	113.80	109.22
1	B	214	UFT	O2-C2-N1	-2.19	119.88	122.79
1	A	353	CFZ	C2'-C1'-N1	-2.18	110.86	114.20
1	B	372	CFZ	C2'-C1'-N1	-2.18	110.86	114.20
1	A	347	UFT	C2'-C1'-N1	-2.18	110.86	114.20
1	A	513	UFT	C2'-C3'-C4'	2.18	105.22	102.40
1	B	536	CFZ	C2'-C1'-N1	-2.18	110.87	114.20
1	B	156	CFZ	O2-C2-N3	-2.18	118.79	122.33
1	B	657	CFZ	F2'-C2'-C3'	2.18	113.78	109.22
1	A	555	UFT	O2-C2-N1	-2.18	119.89	122.79
1	A	712	UFT	C3'-C2'-C1'	2.17	105.76	103.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	574	CFZ	C2'-C3'-C4'	2.17	105.21	102.40
1	A	720	UFT	O2-C2-N1	-2.17	119.90	122.79
1	A	10	CFZ	C2'-C3'-C4'	2.17	105.21	102.40
1	A	80	UFT	C2'-C3'-C4'	2.17	105.21	102.40
1	A	304	CFZ	C3'-C2'-C1'	2.17	105.76	103.13
1	A	614	CFZ	C2'-C3'-C4'	2.17	105.20	102.40
1	A	137	UFT	O2-C2-N1	-2.17	119.91	122.79
1	B	321	CFZ	O4'-C1'-C2'	2.17	108.02	105.79
1	B	254	CFZ	C2'-C3'-C4'	2.17	105.20	102.40
1	A	492	CFZ	C2'-C1'-N1	-2.17	110.89	114.20
1	A	587	CFZ	C2'-C3'-C4'	2.16	105.20	102.40
1	B	165	CFZ	C3'-C2'-C1'	2.16	105.75	103.13
1	B	708	UFT	C3'-C2'-C1'	2.16	105.75	103.13
1	A	610	CFZ	O4'-C1'-C2'	2.16	108.02	105.79
1	B	367	UFT	C3'-C2'-C1'	2.16	105.75	103.13
1	A	530	UFT	C1'-N1-C2	2.16	121.48	117.57
1	A	32	UFT	C2'-C3'-C4'	2.16	105.20	102.40
1	B	142	UFT	O2-C2-N1	-2.16	119.91	122.79
1	B	360	CFZ	C2'-C1'-N1	-2.16	110.90	114.20
1	A	190	UFT	O2-C2-N1	-2.16	119.92	122.79
1	A	657	CFZ	C2'-C1'-N1	-2.16	110.90	114.20
1	A	32	UFT	O2-C2-N1	-2.16	119.92	122.79
1	A	153	UFT	C2'-C3'-C4'	2.16	105.19	102.40
1	B	633	UFT	C3'-C2'-C1'	2.16	105.74	103.13
1	B	647	CFZ	C2'-C3'-C4'	2.16	105.19	102.40
1	A	679	CFZ	C2'-C3'-C4'	2.16	105.19	102.40
1	A	360	CFZ	O4'-C1'-C2'	2.16	108.01	105.79
1	B	549	UFT	C2'-C3'-C4'	2.16	105.19	102.40
1	A	593	UFT	O2-C2-N1	-2.15	119.92	122.79
1	A	355	CFZ	F2'-C2'-C3'	2.15	113.73	109.22
1	A	424	CFZ	O2-C2-N3	-2.15	118.83	122.33
1	A	413	UFT	C3'-C2'-C1'	2.15	105.73	103.13
1	B	417	CFZ	O4'-C1'-C2'	2.15	108.01	105.79
1	A	351	CFZ	C2'-C1'-N1	-2.15	110.92	114.20
1	A	621	UFT	C2'-C1'-N1	-2.15	110.92	114.20
1	A	361	UFT	C1'-N1-C2	2.15	121.46	117.57
1	A	489	UFT	C2'-C1'-N1	-2.15	110.92	114.20
1	B	358	UFT	C1'-N1-C2	2.15	121.46	117.57
1	A	39	CFZ	C3'-C2'-C1'	2.15	105.73	103.13
1	A	372	CFZ	C2'-C1'-N1	-2.14	110.92	114.20
1	A	362	CFZ	O4'-C1'-C2'	2.14	108.00	105.79
1	B	115	UFT	O2-C2-N1	-2.14	119.94	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	CFZ	C2'-C1'-N1	-2.14	110.93	114.20
1	A	367	UFT	C3'-C2'-C1'	2.14	105.72	103.13
1	A	33	UFT	C1'-N1-C2	2.14	121.44	117.57
1	B	313	UFT	C3'-C2'-C1'	2.14	105.72	103.13
1	B	464	UFT	C1'-N1-C2	2.14	121.44	117.57
1	B	313	UFT	C2'-C3'-C4'	2.14	105.16	102.40
1	A	142	UFT	O2-C2-N1	-2.14	119.95	122.79
1	B	565	CFZ	C3'-C2'-C1'	2.14	105.72	103.13
1	A	464	UFT	C1'-N1-C2	2.14	121.44	117.57
1	B	447	UFT	O2-C2-N1	-2.14	119.95	122.79
1	B	13	UFT	O2-C2-N1	-2.13	119.95	122.79
1	B	301	UFT	O2-C2-N1	-2.13	119.95	122.79
1	A	308	CFZ	C2'-C1'-N1	-2.13	110.94	114.20
1	A	336	UFT	O2-C2-N1	-2.13	119.95	122.79
1	A	519	UFT	O2-C2-N1	-2.13	119.95	122.79
1	A	473	CFZ	C2'-C1'-N1	-2.13	110.94	114.20
1	B	499	UFT	C2'-C1'-N1	-2.13	110.94	114.20
1	B	247	CFZ	C2'-C3'-C4'	2.13	105.16	102.40
1	A	363	CFZ	C2'-C3'-C4'	2.13	105.16	102.40
1	B	336	UFT	O2-C2-N1	-2.13	119.96	122.79
1	A	607	UFT	O2-C2-N1	-2.13	119.96	122.79
1	A	329	UFT	C3'-C2'-C1'	2.13	105.71	103.13
1	A	690	UFT	O2-C2-N1	-2.13	119.96	122.79
1	B	282	CFZ	O4'-C1'-C2'	2.13	107.98	105.79
1	A	577	UFT	C3'-C2'-C1'	2.13	105.70	103.13
1	A	114	CFZ	C2'-C1'-N1	-2.13	110.95	114.20
1	A	241	CFZ	C2'-C1'-N1	-2.13	110.95	114.20
1	A	301	UFT	C2'-C1'-N1	-2.13	110.95	114.20
1	B	494	CFZ	C2'-C3'-C4'	2.13	105.15	102.40
1	B	251	UFT	C3'-C2'-C1'	2.12	105.70	103.13
1	B	285	CFZ	C2'-C3'-C4'	2.12	105.15	102.40
1	A	112	UFT	C2'-C3'-C4'	2.12	105.15	102.40
1	A	666	UFT	O2-C2-N1	-2.12	119.97	122.79
1	A	574	CFZ	C2'-C1'-N1	-2.12	110.96	114.20
1	B	518	CFZ	O4'-C1'-C2'	2.12	107.98	105.79
1	B	137	UFT	O2-C2-N1	-2.12	119.97	122.79
1	A	708	UFT	C3'-C2'-C1'	2.12	105.70	103.13
1	A	246	CFZ	C2'-C3'-C4'	2.12	105.14	102.40
1	A	662	UFT	O2-C2-N1	-2.12	119.97	122.79
1	B	308	CFZ	C2'-C1'-N1	-2.12	110.96	114.20
1	B	131	CFZ	C2'-C3'-C4'	2.12	105.14	102.40
1	B	603	CFZ	C2'-C3'-C4'	2.12	105.14	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	629	UFT	O2-C2-N1	-2.12	119.97	122.79
1	B	355	CFZ	C2'-C3'-C4'	2.12	105.14	102.40
1	B	582	UFT	O2-C2-N1	-2.11	119.98	122.79
1	B	662	UFT	O2-C2-N1	-2.11	119.98	122.79
1	B	513	UFT	C1'-N1-C2	2.11	121.39	117.57
1	B	111	CFZ	O4'-C1'-C2'	2.11	107.97	105.79
1	B	114	CFZ	O4'-C1'-C2'	2.11	107.97	105.79
1	B	540	CFZ	O2-C2-N3	-2.11	118.90	122.33
1	B	653	UFT	O2-C2-N1	-2.11	119.98	122.79
1	B	270	UFT	C2'-C1'-N1	-2.11	110.98	114.20
1	B	621	UFT	O2-C2-N1	-2.11	119.98	122.79
1	A	460	UFT	C2'-C3'-C4'	2.11	105.13	102.40
1	B	11	UFT	O2-C2-N1	-2.11	119.98	122.79
1	B	381	CFZ	C2'-C3'-C4'	2.11	105.12	102.40
1	A	111	CFZ	O4'-C1'-C2'	2.11	107.96	105.79
1	B	215	UFT	O2-C2-N1	-2.11	119.99	122.79
1	B	301	UFT	C2'-C1'-N1	-2.11	110.98	114.20
1	B	241	CFZ	C2'-C1'-N1	-2.11	110.98	114.20
1	B	424	CFZ	O2-C2-N3	-2.10	118.91	122.33
1	B	143	UFT	O2-C2-N1	-2.10	119.99	122.79
1	A	155	UFT	O2-C2-N1	-2.10	119.99	122.79
1	B	637	CFZ	O4'-C1'-C2'	2.10	107.96	105.79
1	A	143	UFT	O2-C2-N1	-2.10	119.99	122.79
1	B	628	UFT	O2-C2-N1	-2.10	119.99	122.79
1	B	322	UFT	C2'-C3'-C4'	2.10	105.12	102.40
1	A	13	UFT	O2-C2-N1	-2.10	119.99	122.79
1	B	101	UFT	O2-C2-N1	-2.10	119.99	122.79
1	A	430	UFT	O2-C2-N1	-2.10	119.99	122.79
1	A	653	UFT	O2-C2-N1	-2.10	119.99	122.79
1	B	313	UFT	O2-C2-N1	-2.10	119.99	122.79
1	A	347	UFT	O2-C2-N1	-2.10	119.99	122.79
1	A	696	UFT	O2-C2-N1	-2.10	119.99	122.79
1	B	460	UFT	C2'-C3'-C4'	2.10	105.12	102.40
1	B	355	CFZ	O2-C2-N3	-2.10	118.92	122.33
1	A	637	CFZ	O4'-C1'-C2'	2.10	107.95	105.79
1	A	74	UFT	O2-C2-N1	-2.10	120.00	122.79
1	B	329	UFT	C3'-C2'-C1'	2.10	105.67	103.13
1	B	363	CFZ	C3'-C2'-C1'	2.10	105.67	103.13
1	A	621	UFT	O2-C2-N1	-2.10	120.00	122.79
1	B	438	CFZ	O4'-C1'-C2'	2.10	107.95	105.79
1	B	155	UFT	O2-C2-N1	-2.10	120.00	122.79
1	B	197	UFT	O2-C2-N1	-2.10	120.00	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	695	UFT	C2'-C3'-C4'	2.10	105.11	102.40
1	A	101	UFT	C2'-C1'-N1	-2.10	111.00	114.20
1	B	39	CFZ	C3'-C2'-C1'	2.10	105.67	103.13
1	B	577	UFT	O2-C2-N1	-2.10	120.00	122.79
1	B	690	UFT	O2-C2-N1	-2.10	120.00	122.79
1	B	491	CFZ	C4'-O4'-C1'	-2.10	104.85	109.47
1	A	60	UFT	O2-C2-N1	-2.10	120.00	122.79
1	B	565	CFZ	C2'-C3'-C4'	2.10	105.11	102.40
1	A	447	UFT	O2-C2-N1	-2.10	120.00	122.79
1	B	491	CFZ	O2-C2-N3	-2.09	118.92	122.33
1	A	493	UFT	O2-C2-N1	-2.09	120.00	122.79
1	B	593	UFT	O2-C2-N1	-2.09	120.00	122.79
1	B	353	CFZ	O4'-C1'-C2'	2.09	107.95	105.79
1	A	94	UFT	C2'-C1'-N1	-2.09	111.00	114.20
1	A	202	UFT	C2'-C1'-N1	-2.09	111.00	114.20
1	A	540	CFZ	O2-C2-N3	-2.09	118.93	122.33
1	B	89	UFT	O2-C2-N1	-2.09	120.01	122.79
1	B	608	UFT	O2-C2-N1	-2.09	120.01	122.79
1	B	466	UFT	C2'-C1'-N1	-2.09	111.00	114.20
1	B	485	UFT	O2-C2-N1	-2.09	120.01	122.79
1	A	582	UFT	O2-C2-N1	-2.09	120.01	122.79
1	A	663	UFT	O2-C2-N1	-2.09	120.01	122.79
1	A	500	UFT	O2-C2-N1	-2.09	120.01	122.79
1	A	577	UFT	O2-C2-N1	-2.09	120.01	122.79
1	B	493	UFT	O4'-C1'-C2'	-2.09	103.64	105.79
1	B	61	UFT	O2-C2-N1	-2.09	120.01	122.79
1	A	89	UFT	O2-C2-N1	-2.09	120.01	122.79
1	A	285	CFZ	C3'-C2'-C1'	2.09	105.66	103.13
1	A	141	UFT	C2'-C1'-N1	-2.09	111.01	114.20
1	B	94	UFT	O2-C2-N1	-2.09	120.01	122.79
1	A	200	UFT	O2-C2-N1	-2.09	120.01	122.79
1	B	657	CFZ	C2'-C1'-N1	-2.08	111.02	114.20
1	A	69	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	116	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	190	UFT	O2-C2-N1	-2.08	120.02	122.79
1	A	629	UFT	O2-C2-N1	-2.08	120.02	122.79
1	A	79	CFZ	C2'-C1'-N1	-2.08	111.02	114.20
1	A	565	CFZ	C2'-C3'-C4'	2.08	105.09	102.40
1	A	503	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	666	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	631	CFZ	O4'-C1'-C2'	2.08	107.94	105.79
1	A	304	CFZ	C2'-C3'-C4'	2.08	105.09	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	UFT	O2-C2-N1	-2.08	120.02	122.79
1	A	530	UFT	C2'-C1'-N1	-2.08	111.02	114.20
1	B	550	CFZ	C2'-C3'-C4'	2.08	105.09	102.40
1	A	197	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	96	CFZ	O4'-C1'-C2'	2.08	107.93	105.79
1	B	695	UFT	C2'-C3'-C4'	2.08	105.09	102.40
1	A	61	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	112	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	163	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	437	UFT	O2-C2-N1	-2.08	120.02	122.79
1	A	296	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	296	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	696	UFT	O2-C2-N1	-2.08	120.02	122.79
1	B	719	UFT	O2-C2-N1	-2.08	120.02	122.79
1	A	565	CFZ	C3'-C2'-C1'	2.08	105.65	103.13
1	A	270	UFT	C2'-C1'-N1	-2.08	111.03	114.20
1	B	609	UFT	O2-C2-N1	-2.08	120.03	122.79
1	B	663	UFT	O2-C2-N1	-2.08	120.03	122.79
1	B	192	UFT	C3'-C2'-C1'	2.08	105.64	103.13
1	A	471	UFT	O2-C2-N1	-2.07	120.03	122.79
1	B	655	CFZ	O4'-C1'-C2'	2.07	107.93	105.79
1	A	8	UFT	C2'-C3'-C4'	2.07	105.08	102.40
1	A	160	UFT	O2-C2-N1	-2.07	120.03	122.79
1	A	609	UFT	O2-C2-N1	-2.07	120.03	122.79
1	B	153	UFT	C2'-C3'-C4'	2.07	105.08	102.40
1	B	308	CFZ	O4'-C1'-C2'	2.07	107.93	105.79
1	B	251	UFT	O2-C2-N1	-2.07	120.03	122.79
1	A	28	CFZ	O4'-C1'-N1	2.07	113.10	108.36
1	B	62	UFT	O2-C2-N1	-2.07	120.03	122.79
1	A	217	UFT	O2-C2-N1	-2.07	120.03	122.79
1	A	398	UFT	O2-C2-N1	-2.07	120.03	122.79
1	B	200	UFT	O2-C2-N1	-2.07	120.03	122.79
1	A	389	UFT	C2'-C3'-C4'	2.07	105.08	102.40
1	B	233	UFT	C2'-C3'-C4'	2.07	105.08	102.40
1	A	265	UFT	C2'-C1'-N1	-2.07	111.04	114.20
1	A	25	CFZ	O4'-C1'-C2'	2.07	107.92	105.79
1	B	217	UFT	O2-C2-N1	-2.07	120.04	122.79
1	B	141	UFT	C2'-C1'-N1	-2.07	111.04	114.20
1	A	114	CFZ	O4'-C1'-C2'	2.07	107.92	105.79
1	A	438	CFZ	O4'-C1'-C2'	2.07	107.92	105.79
1	A	687	UFT	O2-C2-N1	-2.07	120.04	122.79
1	A	251	UFT	O2-C2-N1	-2.07	120.04	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	500	UFT	O2-C2-N1	-2.07	120.04	122.79
1	A	131	CFZ	C2'-C3'-C4'	2.07	105.07	102.40
1	A	124	CFZ	C3'-C2'-C1'	2.07	105.63	103.13
1	A	62	UFT	O2-C2-N1	-2.07	120.04	122.79
1	A	112	UFT	O2-C2-N1	-2.07	120.04	122.79
1	A	404	CFZ	C4'-O4'-C1'	-2.06	104.92	109.47
1	A	430	UFT	C2'-C1'-N1	-2.06	111.05	114.20
1	A	554	UFT	O2-C2-N1	-2.06	120.04	122.79
1	A	116	UFT	O2-C2-N1	-2.06	120.04	122.79
1	B	687	UFT	O2-C2-N1	-2.06	120.04	122.79
1	B	46	CFZ	C3'-C2'-C1'	2.06	105.63	103.13
1	B	160	UFT	O2-C2-N1	-2.06	120.04	122.79
1	B	285	CFZ	C3'-C2'-C1'	2.06	105.63	103.13
1	B	359	UFT	C2'-C3'-C4'	2.06	105.07	102.40
1	A	71	UFT	O2-C2-N1	-2.06	120.05	122.79
1	B	182	UFT	C2'-C1'-N1	-2.06	111.05	114.20
1	A	655	CFZ	O4'-C1'-C2'	2.06	107.91	105.79
1	A	308	CFZ	O4'-C1'-C2'	2.06	107.91	105.79
1	A	606	UFT	O2-C2-N1	-2.06	120.05	122.79
1	A	101	UFT	O2-C2-N1	-2.06	120.05	122.79
1	A	583	CFZ	O4'-C1'-C2'	2.06	107.91	105.79
1	A	466	UFT	C2'-C1'-N1	-2.06	111.06	114.20
1	A	163	UFT	O2-C2-N1	-2.06	120.05	122.79
1	A	656	UFT	O2-C2-N1	-2.06	120.05	122.79
1	A	551	CFZ	C3'-C2'-C1'	2.06	105.62	103.13
1	B	182	UFT	O2-C2-N1	-2.06	120.05	122.79
1	A	11	UFT	O2-C2-N1	-2.05	120.06	122.79
1	A	285	CFZ	C2'-C3'-C4'	2.05	105.06	102.40
1	A	628	UFT	O2-C2-N1	-2.05	120.06	122.79
1	A	260	UFT	C3'-C2'-C1'	2.05	105.62	103.13
1	B	60	UFT	O4'-C1'-C2'	2.05	107.91	105.79
1	B	377	UFT	C1'-N1-C2	2.05	121.28	117.57
1	B	86	UFT	C2'-C3'-C4'	2.05	105.05	102.40
1	A	459	CFZ	O4'-C1'-C2'	2.05	107.91	105.79
1	A	57	CFZ	C2'-C3'-C4'	2.05	105.05	102.40
1	B	576	CFZ	O4'-C1'-C2'	2.05	107.90	105.79
1	A	403	UFT	O2-C2-N1	-2.05	120.06	122.79
1	B	656	UFT	O2-C2-N1	-2.05	120.06	122.79
1	A	377	UFT	C1'-N1-C2	2.05	121.28	117.57
1	B	504	UFT	O2-C2-N1	-2.05	120.06	122.79
1	B	398	UFT	O2-C2-N1	-2.05	120.06	122.79
1	A	631	CFZ	O4'-C1'-C2'	2.05	107.90	105.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	CFZ	C4'-O4'-C1'	-2.05	104.96	109.47
1	B	344	UFT	C3'-C2'-C1'	2.04	105.61	103.13
1	A	698	CFZ	C2'-C3'-C4'	2.04	105.04	102.40
1	A	350	UFT	O2-C2-N1	-2.04	120.07	122.79
1	A	543	CFZ	O4'-C1'-C2'	2.04	107.90	105.79
1	B	71	UFT	O2-C2-N1	-2.04	120.07	122.79
1	A	604	CFZ	C4'-O4'-C1'	-2.04	104.97	109.47
1	A	196	UFT	C2'-C1'-N1	-2.04	111.08	114.20
1	B	352	UFT	C2'-C1'-N1	-2.04	111.08	114.20
1	B	473	CFZ	C2'-C1'-N1	-2.04	111.08	114.20
1	B	698	CFZ	C2'-C3'-C4'	2.04	105.04	102.40
1	B	117	CFZ	O4'-C1'-C2'	2.04	107.89	105.79
1	A	171	CFZ	O4'-C1'-C2'	2.04	107.89	105.79
1	A	358	UFT	C2'-C1'-N1	-2.04	111.08	114.20
1	B	170	UFT	O2-C2-N1	-2.04	120.08	122.79
1	A	504	UFT	O2-C2-N1	-2.04	120.08	122.79
1	A	214	UFT	C2'-C3'-C4'	2.04	105.04	102.40
1	A	635	UFT	O2-C2-N1	-2.04	120.08	122.79
1	A	440	CFZ	O4'-C1'-C2'	2.04	107.89	105.79
1	B	606	UFT	O4'-C1'-C2'	2.04	107.89	105.79
1	A	542	UFT	O2-C2-N1	-2.03	120.08	122.79
1	B	329	UFT	O2-C2-N1	-2.03	120.08	122.79
1	B	554	UFT	O2-C2-N1	-2.03	120.08	122.79
1	A	383	CFZ	C2'-C1'-N1	-2.03	111.09	114.20
1	A	513	UFT	C1'-N1-C2	2.03	121.25	117.57
1	B	249	CFZ	C2'-C3'-C4'	2.03	105.03	102.40
1	B	712	UFT	C3'-C2'-C1'	2.03	105.59	103.13
1	B	60	UFT	O2-C2-N1	-2.03	120.09	122.79
1	A	44	UFT	C2'-C3'-C4'	2.03	105.03	102.40
1	B	260	UFT	C3'-C2'-C1'	2.03	105.59	103.13
1	B	460	UFT	C3'-C2'-C1'	2.03	105.59	103.13
1	A	608	UFT	O2-C2-N1	-2.03	120.09	122.79
1	B	196	UFT	C2'-C1'-N1	-2.03	111.10	114.20
1	B	86	UFT	O2-C2-N1	-2.03	120.09	122.79
1	B	88	UFT	O2-C2-N1	-2.03	120.09	122.79
1	A	636	UFT	O2-C2-N1	-2.03	120.09	122.79
1	A	444	CFZ	O4'-C1'-C2'	2.03	107.88	105.79
1	B	49	CFZ	C2'-C3'-C4'	2.03	105.02	102.40
1	A	86	UFT	O2-C2-N1	-2.03	120.09	122.79
1	B	266	UFT	O2-C2-N1	-2.03	120.09	122.79
1	B	583	CFZ	O4'-C1'-C2'	2.03	107.88	105.79
1	A	344	UFT	C2'-C1'-N1	-2.03	111.10	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	UFT	O2-C2-N1	-2.03	120.09	122.79
1	A	455	CFZ	O2-C2-N3	-2.03	119.04	122.33
1	B	636	UFT	O2-C2-N1	-2.03	120.09	122.79
1	B	32	UFT	C2'-C3'-C4'	2.03	105.02	102.40
1	B	466	UFT	O2-C2-N1	-2.03	120.09	122.79
1	B	471	UFT	O2-C2-N1	-2.03	120.09	122.79
1	B	114	CFZ	C2'-C1'-N1	-2.03	111.11	114.20
1	B	447	UFT	C2'-C3'-C4'	2.02	105.02	102.40
1	A	63	CFZ	O4'-C1'-C2'	2.02	107.88	105.79
1	B	309	UFT	O2-C2-N1	-2.02	120.10	122.79
1	B	434	UFT	O2-C2-N1	-2.02	120.10	122.79
1	A	182	UFT	O2-C2-N1	-2.02	120.10	122.79
1	A	88	UFT	O2-C2-N1	-2.02	120.10	122.79
1	B	459	CFZ	O4'-C1'-C2'	2.02	107.87	105.79
1	A	359	UFT	O2-C2-N3	-2.02	117.74	121.50
1	A	431	UFT	O2-C2-N1	-2.02	120.10	122.79
1	A	695	UFT	O2-C2-N1	-2.02	120.10	122.79
1	A	8	UFT	O2-C2-N1	-2.02	120.10	122.79
1	A	104	CFZ	C2'-C3'-C4'	2.02	105.01	102.40
1	A	460	UFT	C3'-C2'-C1'	2.02	105.57	103.13
1	B	473	CFZ	C4'-O4'-C1'	-2.02	105.02	109.47
1	A	97	UFT	O2-C2-N1	-2.02	120.10	122.79
1	A	169	UFT	O2-C2-N1	-2.02	120.10	122.79
1	B	265	UFT	O2-C2-N1	-2.02	120.10	122.79
1	A	349	CFZ	C2'-C3'-C4'	2.02	105.01	102.40
1	B	124	CFZ	C3'-C2'-C1'	2.02	105.57	103.13
1	B	202	UFT	O2-C2-N1	-2.02	120.11	122.79
1	A	618	UFT	O2-C2-N1	-2.02	120.11	122.79
1	A	170	UFT	O2-C2-N1	-2.02	120.11	122.79
1	B	361	UFT	O2-C2-N1	-2.02	120.11	122.79
1	B	587	CFZ	C2'-C3'-C4'	2.02	105.01	102.40
1	B	15	CFZ	C4'-O4'-C1'	-2.02	105.03	109.47
1	A	352	UFT	O2-C2-N1	-2.01	120.11	122.79
1	A	437	UFT	O2-C2-N1	-2.01	120.11	122.79
1	A	387	CFZ	O2-C2-N3	-2.01	119.06	122.33
1	A	249	CFZ	C2'-C3'-C4'	2.01	105.00	102.40
1	B	610	CFZ	O4'-C1'-C2'	2.01	107.86	105.79
1	B	519	UFT	O2-C2-N1	-2.01	120.11	122.79
1	A	602	UFT	O2-C2-N1	-2.01	120.11	122.79
1	B	430	UFT	O2-C2-N1	-2.01	120.11	122.79
1	A	208	UFT	O2-C2-N1	-2.01	120.11	122.79
1	A	309	UFT	O2-C2-N1	-2.01	120.11	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	695	UFT	O2-C2-N1	-2.01	120.11	122.79
1	B	63	CFZ	O4'-C1'-C2'	2.01	107.86	105.79
1	B	171	CFZ	O4'-C1'-C2'	2.01	107.86	105.79
1	B	328	CFZ	O4'-C1'-C2'	2.01	107.86	105.79
1	A	50	UFT	C3'-C2'-C1'	2.01	105.56	103.13
1	A	92	UFT	C3'-C2'-C1'	2.01	105.56	103.13
1	B	21	CFZ	C2'-C3'-C4'	2.00	104.99	102.40
1	A	447	UFT	C2'-C3'-C4'	2.00	104.99	102.40
1	A	684	UFT	C3'-C2'-C1'	2.00	105.56	103.13
1	A	15	CFZ	C4'-O4'-C1'	-2.00	105.05	109.47
1	B	98	UFT	O2-C2-N1	-2.00	120.12	122.79
1	B	618	UFT	O2-C2-N1	-2.00	120.12	122.79
1	A	117	CFZ	O4'-C1'-C2'	2.00	107.86	105.79
1	A	212	CFZ	O4'-C1'-C2'	2.00	107.86	105.79
1	B	169	UFT	O2-C2-N1	-2.00	120.12	122.79
1	A	434	UFT	O2-C2-N1	-2.00	120.12	122.79
1	A	517	CFZ	O4'-C1'-C2'	2.00	107.86	105.79
1	A	208	UFT	C2'-C1'-N1	-2.00	111.14	114.20
1	B	556	CFZ	C2'-C1'-N1	-2.00	111.14	114.20
1	B	635	UFT	O2-C2-N1	-2.00	120.12	122.79
1	B	359	UFT	O2-C2-N1	-2.00	120.13	122.79
1	B	403	UFT	O2-C2-N1	-2.00	120.13	122.79
1	A	245	UFT	O2-C2-N1	-2.00	120.13	122.79
1	B	270	UFT	O2-C2-N1	-2.00	120.13	122.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	720	UFT	C2'

All (709) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	8	UFT	O4'-C4'-C5'-O5'
1	B	8	UFT	C3'-C4'-C5'-O5'
1	A	10	CFZ	C3'-C4'-C5'-O5'
1	A	15	CFZ	C3'-C4'-C5'-O5'
1	B	15	CFZ	C3'-C4'-C5'-O5'
1	A	19	UFT	C3'-C4'-C5'-O5'
1	B	19	UFT	C3'-C4'-C5'-O5'
1	B	25	CFZ	C3'-C4'-C5'-O5'
1	A	32	UFT	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	32	UFT	C3'-C4'-C5'-O5'
1	B	32	UFT	C3'-C4'-C5'-O5'
1	A	43	UFT	O4'-C1'-N1-C6
1	A	43	UFT	O4'-C1'-N1-C2
1	A	43	UFT	C3'-C4'-C5'-O5'
1	B	43	UFT	O4'-C1'-N1-C6
1	B	43	UFT	O4'-C1'-N1-C2
1	B	43	UFT	C3'-C4'-C5'-O5'
1	A	44	UFT	O4'-C4'-C5'-O5'
1	B	44	UFT	O4'-C4'-C5'-O5'
1	A	46	CFZ	C3'-C4'-C5'-O5'
1	B	57	CFZ	C3'-C4'-C5'-O5'
1	B	57	CFZ	O4'-C4'-C5'-O5'
1	B	60	UFT	O4'-C4'-C5'-O5'
1	B	60	UFT	C3'-C4'-C5'-O5'
1	A	67	CFZ	C3'-C4'-C5'-O5'
1	A	71	UFT	O4'-C4'-C5'-O5'
1	A	76	CFZ	C3'-C4'-C5'-O5'
1	B	76	CFZ	C3'-C4'-C5'-O5'
1	A	80	UFT	C3'-C4'-C5'-O5'
1	B	80	UFT	C3'-C4'-C5'-O5'
1	A	84	UFT	O4'-C4'-C5'-O5'
1	A	84	UFT	C3'-C4'-C5'-O5'
1	A	88	UFT	O4'-C4'-C5'-O5'
1	A	88	UFT	C3'-C4'-C5'-O5'
1	B	88	UFT	O4'-C4'-C5'-O5'
1	B	88	UFT	C3'-C4'-C5'-O5'
1	A	92	UFT	O4'-C4'-C5'-O5'
1	A	92	UFT	C3'-C4'-C5'-O5'
1	B	92	UFT	O4'-C4'-C5'-O5'
1	B	92	UFT	C3'-C4'-C5'-O5'
1	A	106	UFT	C4'-C5'-O5'-P
1	A	106	UFT	C3'-C4'-C5'-O5'
1	B	106	UFT	C4'-C5'-O5'-P
1	B	106	UFT	C3'-C4'-C5'-O5'
1	A	108	UFT	O4'-C4'-C5'-O5'
1	A	108	UFT	C3'-C4'-C5'-O5'
1	B	108	UFT	O4'-C4'-C5'-O5'
1	B	108	UFT	C3'-C4'-C5'-O5'
1	A	120	CFZ	C3'-C4'-C5'-O5'
1	A	120	CFZ	O4'-C4'-C5'-O5'
1	B	120	CFZ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B	120	CFZ	O4'-C4'-C5'-O5'
1	A	124	CFZ	C3'-C4'-C5'-O5'
1	A	124	CFZ	O4'-C4'-C5'-O5'
1	B	124	CFZ	C3'-C4'-C5'-O5'
1	B	124	CFZ	O4'-C4'-C5'-O5'
1	A	143	UFT	C3'-C4'-C5'-O5'
1	B	143	UFT	C3'-C4'-C5'-O5'
1	A	144	CFZ	O4'-C4'-C5'-O5'
1	B	144	CFZ	O4'-C4'-C5'-O5'
1	A	151	CFZ	C3'-C4'-C5'-O5'
1	B	151	CFZ	C3'-C4'-C5'-O5'
1	A	171	CFZ	O4'-C4'-C5'-O5'
1	B	171	CFZ	O4'-C4'-C5'-O5'
1	A	173	CFZ	O4'-C4'-C5'-O5'
1	B	173	CFZ	O4'-C4'-C5'-O5'
1	A	175	UFT	O4'-C4'-C5'-O5'
1	A	175	UFT	C3'-C4'-C5'-O5'
1	B	175	UFT	O4'-C4'-C5'-O5'
1	B	175	UFT	C3'-C4'-C5'-O5'
1	A	184	CFZ	C3'-C4'-C5'-O5'
1	A	184	CFZ	O4'-C4'-C5'-O5'
1	B	184	CFZ	C3'-C4'-C5'-O5'
1	B	184	CFZ	O4'-C4'-C5'-O5'
1	A	188	CFZ	C3'-C4'-C5'-O5'
1	B	188	CFZ	C3'-C4'-C5'-O5'
1	A	196	UFT	O4'-C1'-N1-C2
1	B	196	UFT	O4'-C1'-N1-C2
1	A	201	CFZ	C3'-C4'-C5'-O5'
1	B	201	CFZ	C3'-C4'-C5'-O5'
1	B	202	UFT	O4'-C4'-C5'-O5'
1	B	202	UFT	C3'-C4'-C5'-O5'
1	B	206	CFZ	C3'-C4'-C5'-O5'
1	A	229	UFT	C3'-C4'-C5'-O5'
1	B	229	UFT	O4'-C4'-C5'-O5'
1	B	229	UFT	C3'-C4'-C5'-O5'
1	A	232	CFZ	C3'-C4'-C5'-O5'
1	A	232	CFZ	O4'-C4'-C5'-O5'
1	B	233	UFT	C3'-C4'-C5'-O5'
1	A	234	CFZ	C3'-C4'-C5'-O5'
1	A	234	CFZ	O4'-C4'-C5'-O5'
1	A	234	CFZ	C4'-C5'-O5'-P
1	B	234	CFZ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B	234	CFZ	O4'-C4'-C5'-O5'
1	B	234	CFZ	C4'-C5'-O5'-P
1	A	241	CFZ	C3'-C4'-C5'-O5'
1	A	251	UFT	O4'-C4'-C5'-O5'
1	A	251	UFT	C3'-C4'-C5'-O5'
1	B	251	UFT	O4'-C4'-C5'-O5'
1	B	251	UFT	C3'-C4'-C5'-O5'
1	A	283	UFT	O4'-C4'-C5'-O5'
1	A	283	UFT	C3'-C4'-C5'-O5'
1	B	283	UFT	O4'-C4'-C5'-O5'
1	B	283	UFT	C3'-C4'-C5'-O5'
1	A	293	UFT	O4'-C4'-C5'-O5'
1	A	293	UFT	C3'-C4'-C5'-O5'
1	B	293	UFT	O4'-C4'-C5'-O5'
1	B	293	UFT	C3'-C4'-C5'-O5'
1	A	305	UFT	O4'-C4'-C5'-O5'
1	A	305	UFT	C3'-C4'-C5'-O5'
1	B	305	UFT	O4'-C4'-C5'-O5'
1	B	305	UFT	C3'-C4'-C5'-O5'
1	B	322	UFT	C3'-C4'-C5'-O5'
1	A	325	CFZ	C3'-C4'-C5'-O5'
1	A	328	CFZ	C3'-C4'-C5'-O5'
1	A	328	CFZ	O4'-C4'-C5'-O5'
1	A	328	CFZ	C4'-C5'-O5'-P
1	B	328	CFZ	C3'-C4'-C5'-O5'
1	B	328	CFZ	O4'-C4'-C5'-O5'
1	B	328	CFZ	C4'-C5'-O5'-P
1	A	329	UFT	O4'-C4'-C5'-O5'
1	A	329	UFT	C3'-C4'-C5'-O5'
1	B	329	UFT	O4'-C4'-C5'-O5'
1	B	329	UFT	C3'-C4'-C5'-O5'
1	A	335	CFZ	C3'-C4'-C5'-O5'
1	A	335	CFZ	O4'-C4'-C5'-O5'
1	B	335	CFZ	C3'-C4'-C5'-O5'
1	B	335	CFZ	O4'-C4'-C5'-O5'
1	B	338	CFZ	C3'-C4'-C5'-O5'
1	B	338	CFZ	O4'-C4'-C5'-O5'
1	A	344	UFT	C3'-C4'-C5'-O5'
1	B	344	UFT	O4'-C4'-C5'-O5'
1	B	344	UFT	C3'-C4'-C5'-O5'
1	A	349	CFZ	O4'-C4'-C5'-O5'
1	A	354	CFZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B	354	CFZ	C3'-C4'-C5'-O5'
1	B	355	CFZ	C3'-C4'-C5'-O5'
1	B	355	CFZ	O4'-C4'-C5'-O5'
1	B	361	UFT	C3'-C4'-C5'-O5'
1	B	363	CFZ	O4'-C4'-C5'-O5'
1	A	367	UFT	C3'-C4'-C5'-O5'
1	B	367	UFT	C3'-C4'-C5'-O5'
1	A	377	UFT	C3'-C4'-C5'-O5'
1	B	377	UFT	C3'-C4'-C5'-O5'
1	A	382	CFZ	C3'-C4'-C5'-O5'
1	A	382	CFZ	O4'-C4'-C5'-O5'
1	A	383	CFZ	C3'-C4'-C5'-O5'
1	B	384	CFZ	C3'-C4'-C5'-O5'
1	B	384	CFZ	C4'-C5'-O5'-P
1	B	387	CFZ	C3'-C4'-C5'-O5'
1	B	387	CFZ	O4'-C4'-C5'-O5'
1	A	413	UFT	C3'-C4'-C5'-O5'
1	A	423	UFT	C3'-C4'-C5'-O5'
1	B	423	UFT	C3'-C4'-C5'-O5'
1	A	441	CFZ	C3'-C4'-C5'-O5'
1	A	441	CFZ	O4'-C4'-C5'-O5'
1	A	460	UFT	C3'-C4'-C5'-O5'
1	B	460	UFT	C3'-C4'-C5'-O5'
1	B	464	UFT	C3'-C4'-C5'-O5'
1	A	472	UFT	O4'-C4'-C5'-O5'
1	A	472	UFT	C3'-C4'-C5'-O5'
1	B	472	UFT	C3'-C4'-C5'-O5'
1	B	474	CFZ	O4'-C4'-C5'-O5'
1	A	477	CFZ	C3'-C4'-C5'-O5'
1	A	477	CFZ	O4'-C4'-C5'-O5'
1	B	477	CFZ	C3'-C4'-C5'-O5'
1	B	477	CFZ	O4'-C4'-C5'-O5'
1	B	485	UFT	C3'-C4'-C5'-O5'
1	B	486	CFZ	C2'-C1'-N1-C2
1	B	486	CFZ	C2'-C1'-N1-C6
1	B	491	CFZ	C3'-C4'-C5'-O5'
1	B	491	CFZ	O4'-C4'-C5'-O5'
1	B	493	UFT	C2'-C1'-N1-C2
1	A	502	UFT	O4'-C4'-C5'-O5'
1	A	502	UFT	C3'-C4'-C5'-O5'
1	B	502	UFT	O4'-C4'-C5'-O5'
1	B	502	UFT	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	503	UFT	O4'-C4'-C5'-O5'
1	A	503	UFT	C3'-C4'-C5'-O5'
1	A	504	UFT	O4'-C4'-C5'-O5'
1	A	504	UFT	C3'-C4'-C5'-O5'
1	B	504	UFT	O4'-C4'-C5'-O5'
1	B	504	UFT	C3'-C4'-C5'-O5'
1	A	519	UFT	O4'-C4'-C5'-O5'
1	A	523	CFZ	C3'-C4'-C5'-O5'
1	A	523	CFZ	O4'-C4'-C5'-O5'
1	B	524	UFT	C4'-C5'-O5'-P
1	B	530	UFT	C3'-C4'-C5'-O5'
1	A	534	UFT	O4'-C4'-C5'-O5'
1	A	534	UFT	C3'-C4'-C5'-O5'
1	B	534	UFT	O4'-C4'-C5'-O5'
1	B	534	UFT	C3'-C4'-C5'-O5'
1	B	544	UFT	C3'-C4'-C5'-O5'
1	A	545	UFT	C3'-C4'-C5'-O5'
1	B	545	UFT	C3'-C4'-C5'-O5'
1	B	554	UFT	O4'-C4'-C5'-O5'
1	B	554	UFT	C3'-C4'-C5'-O5'
1	A	555	UFT	O4'-C4'-C5'-O5'
1	B	555	UFT	O4'-C4'-C5'-O5'
1	A	556	CFZ	C2'-C1'-N1-C2
1	A	556	CFZ	C2'-C1'-N1-C6
1	B	556	CFZ	C2'-C1'-N1-C2
1	B	556	CFZ	C2'-C1'-N1-C6
1	B	558	CFZ	O4'-C4'-C5'-O5'
1	A	564	CFZ	C3'-C4'-C5'-O5'
1	B	564	CFZ	C3'-C4'-C5'-O5'
1	A	565	CFZ	C3'-C4'-C5'-O5'
1	A	565	CFZ	O4'-C4'-C5'-O5'
1	B	565	CFZ	C3'-C4'-C5'-O5'
1	B	565	CFZ	O4'-C4'-C5'-O5'
1	A	571	UFT	C3'-C4'-C5'-O5'
1	B	571	UFT	C3'-C4'-C5'-O5'
1	A	582	UFT	C3'-C4'-C5'-O5'
1	B	582	UFT	C3'-C4'-C5'-O5'
1	A	587	CFZ	O4'-C4'-C5'-O5'
1	A	590	UFT	C4'-C5'-O5'-P
1	B	593	UFT	C3'-C4'-C5'-O5'
1	A	606	UFT	O4'-C4'-C5'-O5'
1	A	606	UFT	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	607	UFT	O4'-C4'-C5'-O5'
1	A	607	UFT	C3'-C4'-C5'-O5'
1	B	607	UFT	C3'-C4'-C5'-O5'
1	A	608	UFT	O4'-C4'-C5'-O5'
1	B	608	UFT	O4'-C4'-C5'-O5'
1	A	610	CFZ	C3'-C4'-C5'-O5'
1	A	610	CFZ	O4'-C4'-C5'-O5'
1	B	614	CFZ	C3'-C4'-C5'-O5'
1	B	614	CFZ	O4'-C4'-C5'-O5'
1	A	637	CFZ	O4'-C4'-C5'-O5'
1	B	637	CFZ	O4'-C4'-C5'-O5'
1	A	639	CFZ	C3'-C4'-C5'-O5'
1	A	639	CFZ	O4'-C4'-C5'-O5'
1	B	639	CFZ	C3'-C4'-C5'-O5'
1	B	639	CFZ	O4'-C4'-C5'-O5'
1	A	657	CFZ	C3'-C4'-C5'-O5'
1	B	657	CFZ	C3'-C4'-C5'-O5'
1	B	657	CFZ	O4'-C4'-C5'-O5'
1	A	659	UFT	C3'-C4'-C5'-O5'
1	B	659	UFT	C3'-C4'-C5'-O5'
1	A	662	UFT	O4'-C4'-C5'-O5'
1	B	662	UFT	O4'-C4'-C5'-O5'
1	A	666	UFT	O4'-C4'-C5'-O5'
1	A	666	UFT	C3'-C4'-C5'-O5'
1	B	666	UFT	O4'-C4'-C5'-O5'
1	B	666	UFT	C3'-C4'-C5'-O5'
1	B	669	UFT	O4'-C4'-C5'-O5'
1	B	669	UFT	C3'-C4'-C5'-O5'
1	A	700	CFZ	C3'-C4'-C5'-O5'
1	A	700	CFZ	O4'-C4'-C5'-O5'
1	B	700	CFZ	C3'-C4'-C5'-O5'
1	A	703	UFT	C3'-C4'-C5'-O5'
1	B	703	UFT	C3'-C4'-C5'-O5'
1	B	704	CFZ	C3'-C4'-C5'-O5'
1	A	712	UFT	C3'-C4'-C5'-O5'
1	B	712	UFT	O4'-C4'-C5'-O5'
1	B	719	UFT	O4'-C4'-C5'-O5'
1	B	719	UFT	C3'-C4'-C5'-O5'
1	A	720	UFT	C3'-C4'-C5'-O5'
1	B	720	UFT	C4'-C5'-O5'-P
1	B	720	UFT	O4'-C4'-C5'-O5'
1	B	720	UFT	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	196	UFT	O4'-C1'-N1-C6
1	B	196	UFT	O4'-C1'-N1-C6
1	A	359	UFT	C4'-C5'-O5'-P
1	A	10	CFZ	O4'-C4'-C5'-O5'
1	A	15	CFZ	O4'-C4'-C5'-O5'
1	B	15	CFZ	O4'-C4'-C5'-O5'
1	A	19	UFT	O4'-C4'-C5'-O5'
1	B	19	UFT	O4'-C4'-C5'-O5'
1	B	25	CFZ	O4'-C4'-C5'-O5'
1	B	32	UFT	O4'-C4'-C5'-O5'
1	A	33	UFT	C3'-C4'-C5'-O5'
1	B	44	UFT	C3'-C4'-C5'-O5'
1	A	46	CFZ	O4'-C4'-C5'-O5'
1	B	46	CFZ	C3'-C4'-C5'-O5'
1	A	49	CFZ	O4'-C4'-C5'-O5'
1	A	63	CFZ	O4'-C4'-C5'-O5'
1	B	63	CFZ	O4'-C4'-C5'-O5'
1	A	67	CFZ	O4'-C4'-C5'-O5'
1	B	67	CFZ	O4'-C4'-C5'-O5'
1	A	71	UFT	C3'-C4'-C5'-O5'
1	A	74	UFT	O4'-C4'-C5'-O5'
1	A	74	UFT	C3'-C4'-C5'-O5'
1	A	76	CFZ	O4'-C4'-C5'-O5'
1	B	76	CFZ	O4'-C4'-C5'-O5'
1	A	80	UFT	O4'-C4'-C5'-O5'
1	B	80	UFT	O4'-C4'-C5'-O5'
1	B	84	UFT	O4'-C4'-C5'-O5'
1	B	84	UFT	C3'-C4'-C5'-O5'
1	A	101	UFT	O4'-C4'-C5'-O5'
1	A	101	UFT	C3'-C4'-C5'-O5'
1	A	110	CFZ	C3'-C4'-C5'-O5'
1	B	110	CFZ	C3'-C4'-C5'-O5'
1	A	117	CFZ	O4'-C4'-C5'-O5'
1	B	117	CFZ	O4'-C4'-C5'-O5'
1	A	143	UFT	O4'-C4'-C5'-O5'
1	B	143	UFT	O4'-C4'-C5'-O5'
1	A	144	CFZ	C3'-C4'-C5'-O5'
1	B	144	CFZ	C3'-C4'-C5'-O5'
1	A	151	CFZ	O4'-C4'-C5'-O5'
1	B	151	CFZ	O4'-C4'-C5'-O5'
1	A	160	UFT	O4'-C4'-C5'-O5'
1	B	171	CFZ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	173	CFZ	C3'-C4'-C5'-O5'
1	B	173	CFZ	C3'-C4'-C5'-O5'
1	A	188	CFZ	O4'-C4'-C5'-O5'
1	B	188	CFZ	O4'-C4'-C5'-O5'
1	B	192	UFT	C3'-C4'-C5'-O5'
1	A	201	CFZ	O4'-C4'-C5'-O5'
1	B	201	CFZ	O4'-C4'-C5'-O5'
1	A	206	CFZ	C3'-C4'-C5'-O5'
1	B	206	CFZ	O4'-C4'-C5'-O5'
1	A	212	CFZ	C3'-C4'-C5'-O5'
1	A	212	CFZ	O4'-C4'-C5'-O5'
1	B	212	CFZ	C3'-C4'-C5'-O5'
1	B	212	CFZ	O4'-C4'-C5'-O5'
1	A	229	UFT	O4'-C4'-C5'-O5'
1	B	232	CFZ	C3'-C4'-C5'-O5'
1	A	233	UFT	C3'-C4'-C5'-O5'
1	B	233	UFT	O4'-C4'-C5'-O5'
1	A	241	CFZ	O4'-C4'-C5'-O5'
1	A	266	UFT	C3'-C4'-C5'-O5'
1	A	322	UFT	C3'-C4'-C5'-O5'
1	B	322	UFT	O4'-C4'-C5'-O5'
1	A	325	CFZ	O4'-C4'-C5'-O5'
1	B	325	CFZ	C3'-C4'-C5'-O5'
1	A	347	UFT	O4'-C4'-C5'-O5'
1	B	347	UFT	O4'-C4'-C5'-O5'
1	A	349	CFZ	C3'-C4'-C5'-O5'
1	A	351	CFZ	O4'-C4'-C5'-O5'
1	B	354	CFZ	O4'-C4'-C5'-O5'
1	B	363	CFZ	C3'-C4'-C5'-O5'
1	A	367	UFT	O4'-C4'-C5'-O5'
1	B	367	UFT	O4'-C4'-C5'-O5'
1	A	377	UFT	O4'-C4'-C5'-O5'
1	B	377	UFT	O4'-C4'-C5'-O5'
1	A	383	CFZ	O4'-C4'-C5'-O5'
1	B	384	CFZ	O4'-C4'-C5'-O5'
1	A	405	CFZ	O4'-C4'-C5'-O5'
1	B	405	CFZ	O4'-C4'-C5'-O5'
1	A	413	UFT	O4'-C4'-C5'-O5'
1	A	423	UFT	O4'-C4'-C5'-O5'
1	B	423	UFT	O4'-C4'-C5'-O5'
1	B	441	CFZ	C3'-C4'-C5'-O5'
1	A	460	UFT	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B	460	UFT	O4'-C4'-C5'-O5'
1	B	464	UFT	O4'-C4'-C5'-O5'
1	B	472	UFT	O4'-C4'-C5'-O5'
1	A	473	CFZ	O4'-C4'-C5'-O5'
1	B	474	CFZ	C3'-C4'-C5'-O5'
1	B	485	UFT	O4'-C4'-C5'-O5'
1	B	493	UFT	O4'-C4'-C5'-O5'
1	B	493	UFT	C3'-C4'-C5'-O5'
1	A	506	CFZ	C3'-C4'-C5'-O5'
1	B	524	UFT	C3'-C4'-C5'-O5'
1	B	530	UFT	O4'-C4'-C5'-O5'
1	A	544	UFT	C3'-C4'-C5'-O5'
1	A	545	UFT	O4'-C4'-C5'-O5'
1	B	545	UFT	O4'-C4'-C5'-O5'
1	A	555	UFT	C3'-C4'-C5'-O5'
1	B	555	UFT	C3'-C4'-C5'-O5'
1	A	564	CFZ	O4'-C4'-C5'-O5'
1	B	564	CFZ	O4'-C4'-C5'-O5'
1	A	571	UFT	O4'-C4'-C5'-O5'
1	B	571	UFT	O4'-C4'-C5'-O5'
1	A	582	UFT	O4'-C4'-C5'-O5'
1	B	582	UFT	O4'-C4'-C5'-O5'
1	A	587	CFZ	C3'-C4'-C5'-O5'
1	B	607	UFT	O4'-C4'-C5'-O5'
1	A	608	UFT	C3'-C4'-C5'-O5'
1	A	637	CFZ	C3'-C4'-C5'-O5'
1	B	637	CFZ	C3'-C4'-C5'-O5'
1	A	657	CFZ	O4'-C4'-C5'-O5'
1	A	659	UFT	O4'-C4'-C5'-O5'
1	B	659	UFT	O4'-C4'-C5'-O5'
1	A	662	UFT	C3'-C4'-C5'-O5'
1	B	662	UFT	C3'-C4'-C5'-O5'
1	A	676	UFT	O4'-C4'-C5'-O5'
1	A	676	UFT	C3'-C4'-C5'-O5'
1	B	676	UFT	O4'-C4'-C5'-O5'
1	B	676	UFT	C3'-C4'-C5'-O5'
1	B	700	CFZ	O4'-C4'-C5'-O5'
1	A	703	UFT	O4'-C4'-C5'-O5'
1	B	703	UFT	O4'-C4'-C5'-O5'
1	A	704	CFZ	C3'-C4'-C5'-O5'
1	A	704	CFZ	O4'-C4'-C5'-O5'
1	B	704	CFZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	712	UFT	O4'-C4'-C5'-O5'
1	B	712	UFT	C3'-C4'-C5'-O5'
1	A	720	UFT	O4'-C4'-C5'-O5'
1	A	659	UFT	C4'-C5'-O5'-P
1	B	659	UFT	C4'-C5'-O5'-P
1	A	25	CFZ	O4'-C4'-C5'-O5'
1	A	33	UFT	O4'-C4'-C5'-O5'
1	A	43	UFT	O4'-C4'-C5'-O5'
1	B	43	UFT	O4'-C4'-C5'-O5'
1	A	44	UFT	C3'-C4'-C5'-O5'
1	B	46	CFZ	O4'-C4'-C5'-O5'
1	B	49	CFZ	C3'-C4'-C5'-O5'
1	B	49	CFZ	O4'-C4'-C5'-O5'
1	A	63	CFZ	C3'-C4'-C5'-O5'
1	B	63	CFZ	C3'-C4'-C5'-O5'
1	B	67	CFZ	C3'-C4'-C5'-O5'
1	B	74	UFT	O4'-C4'-C5'-O5'
1	B	97	UFT	O4'-C4'-C5'-O5'
1	B	97	UFT	C3'-C4'-C5'-O5'
1	A	106	UFT	O4'-C4'-C5'-O5'
1	B	106	UFT	O4'-C4'-C5'-O5'
1	A	110	CFZ	O4'-C4'-C5'-O5'
1	B	110	CFZ	O4'-C4'-C5'-O5'
1	A	117	CFZ	C3'-C4'-C5'-O5'
1	B	160	UFT	O4'-C4'-C5'-O5'
1	A	171	CFZ	C3'-C4'-C5'-O5'
1	A	192	UFT	C3'-C4'-C5'-O5'
1	B	192	UFT	O4'-C4'-C5'-O5'
1	A	206	CFZ	O4'-C4'-C5'-O5'
1	B	232	CFZ	O4'-C4'-C5'-O5'
1	A	233	UFT	O4'-C4'-C5'-O5'
1	B	241	CFZ	O4'-C4'-C5'-O5'
1	A	266	UFT	O4'-C4'-C5'-O5'
1	B	266	UFT	C3'-C4'-C5'-O5'
1	A	296	UFT	O4'-C4'-C5'-O5'
1	B	296	UFT	O4'-C4'-C5'-O5'
1	B	309	UFT	C3'-C4'-C5'-O5'
1	A	322	UFT	O4'-C4'-C5'-O5'
1	B	325	CFZ	O4'-C4'-C5'-O5'
1	B	347	UFT	C3'-C4'-C5'-O5'
1	A	405	CFZ	C3'-C4'-C5'-O5'
1	B	441	CFZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	473	CFZ	C3'-C4'-C5'-O5'
1	A	506	CFZ	O4'-C4'-C5'-O5'
1	B	506	CFZ	C3'-C4'-C5'-O5'
1	B	506	CFZ	O4'-C4'-C5'-O5'
1	A	519	UFT	C3'-C4'-C5'-O5'
1	B	524	UFT	O4'-C4'-C5'-O5'
1	A	530	UFT	C3'-C4'-C5'-O5'
1	B	558	CFZ	C3'-C4'-C5'-O5'
1	B	608	UFT	C3'-C4'-C5'-O5'
1	A	719	UFT	O4'-C4'-C5'-O5'
1	A	719	UFT	C3'-C4'-C5'-O5'
1	A	477	CFZ	C4'-C5'-O5'-P
1	B	477	CFZ	C4'-C5'-O5'-P
1	B	117	CFZ	C3'-C4'-C5'-O5'
1	A	160	UFT	C3'-C4'-C5'-O5'
1	B	266	UFT	O4'-C4'-C5'-O5'
1	B	332	CFZ	C3'-C4'-C5'-O5'
1	A	351	CFZ	C3'-C4'-C5'-O5'
1	B	405	CFZ	C3'-C4'-C5'-O5'
1	B	486	CFZ	C3'-C4'-C5'-O5'
1	A	667	CFZ	C3'-C4'-C5'-O5'
1	B	559	UFT	C4'-C5'-O5'-P
1	A	25	CFZ	C3'-C4'-C5'-O5'
1	B	160	UFT	C3'-C4'-C5'-O5'
1	B	241	CFZ	C3'-C4'-C5'-O5'
1	B	296	UFT	C3'-C4'-C5'-O5'
1	A	309	UFT	C3'-C4'-C5'-O5'
1	A	332	CFZ	C3'-C4'-C5'-O5'
1	A	338	CFZ	C3'-C4'-C5'-O5'
1	A	347	UFT	C3'-C4'-C5'-O5'
1	B	352	UFT	C3'-C4'-C5'-O5'
1	A	456	UFT	C3'-C4'-C5'-O5'
1	B	456	UFT	C3'-C4'-C5'-O5'
1	A	464	UFT	C3'-C4'-C5'-O5'
1	A	471	UFT	C3'-C4'-C5'-O5'
1	A	518	CFZ	C3'-C4'-C5'-O5'
1	A	540	CFZ	C3'-C4'-C5'-O5'
1	B	540	CFZ	C3'-C4'-C5'-O5'
1	B	593	UFT	O4'-C4'-C5'-O5'
1	B	609	UFT	C3'-C4'-C5'-O5'
1	A	655	CFZ	C3'-C4'-C5'-O5'
1	B	655	CFZ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	667	CFZ	O4'-C4'-C5'-O5'
1	A	689	UFT	C3'-C4'-C5'-O5'
1	B	689	UFT	C3'-C4'-C5'-O5'
1	A	361	UFT	C4'-C5'-O5'-P
1	A	481	UFT	C4'-C5'-O5'-P
1	B	481	UFT	C4'-C5'-O5'-P
1	A	499	UFT	C4'-C5'-O5'-P
1	B	499	UFT	C4'-C5'-O5'-P
1	A	559	UFT	C4'-C5'-O5'-P
1	A	75	CFZ	O4'-C4'-C5'-O5'
1	B	114	CFZ	C3'-C4'-C5'-O5'
1	A	192	UFT	O4'-C4'-C5'-O5'
1	B	216	UFT	C3'-C4'-C5'-O5'
1	B	270	UFT	O4'-C4'-C5'-O5'
1	A	296	UFT	C3'-C4'-C5'-O5'
1	A	298	CFZ	C3'-C4'-C5'-O5'
1	B	298	CFZ	C3'-C4'-C5'-O5'
1	B	301	UFT	O4'-C4'-C5'-O5'
1	A	302	UFT	O4'-C4'-C5'-O5'
1	B	302	UFT	O4'-C4'-C5'-O5'
1	A	309	UFT	O4'-C4'-C5'-O5'
1	B	309	UFT	O4'-C4'-C5'-O5'
1	B	332	CFZ	O4'-C4'-C5'-O5'
1	A	338	CFZ	O4'-C4'-C5'-O5'
1	A	344	UFT	O4'-C4'-C5'-O5'
1	A	350	UFT	O4'-C4'-C5'-O5'
1	B	361	UFT	O4'-C4'-C5'-O5'
1	B	486	CFZ	O4'-C4'-C5'-O5'
1	A	517	CFZ	C3'-C4'-C5'-O5'
1	A	530	UFT	O4'-C4'-C5'-O5'
1	B	540	CFZ	O4'-C4'-C5'-O5'
1	A	544	UFT	O4'-C4'-C5'-O5'
1	B	544	UFT	O4'-C4'-C5'-O5'
1	A	621	UFT	C3'-C4'-C5'-O5'
1	A	655	CFZ	O4'-C4'-C5'-O5'
1	B	655	CFZ	O4'-C4'-C5'-O5'
1	B	667	CFZ	C3'-C4'-C5'-O5'
1	B	174	UFT	C4'-C5'-O5'-P
1	A	114	CFZ	C3'-C4'-C5'-O5'
1	A	270	UFT	O4'-C4'-C5'-O5'
1	A	301	UFT	O4'-C4'-C5'-O5'
1	A	302	UFT	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B	302	UFT	C3'-C4'-C5'-O5'
1	A	406	CFZ	C3'-C4'-C5'-O5'
1	B	406	CFZ	C3'-C4'-C5'-O5'
1	A	464	UFT	O4'-C4'-C5'-O5'
1	A	518	CFZ	O4'-C4'-C5'-O5'
1	A	540	CFZ	O4'-C4'-C5'-O5'
1	B	621	UFT	C3'-C4'-C5'-O5'
1	A	689	UFT	O4'-C4'-C5'-O5'
1	B	689	UFT	O4'-C4'-C5'-O5'
1	A	25	CFZ	C4'-C5'-O5'-P
1	B	25	CFZ	C4'-C5'-O5'-P
1	A	97	UFT	C4'-C5'-O5'-P
1	B	97	UFT	C4'-C5'-O5'-P
1	A	141	UFT	C4'-C5'-O5'-P
1	B	141	UFT	C4'-C5'-O5'-P
1	A	174	UFT	C4'-C5'-O5'-P
1	B	192	UFT	C4'-C5'-O5'-P
1	A	229	UFT	C4'-C5'-O5'-P
1	A	334	UFT	C4'-C5'-O5'-P
1	B	334	UFT	C4'-C5'-O5'-P
1	A	493	UFT	C4'-C5'-O5'-P
1	A	513	UFT	C4'-C5'-O5'-P
1	B	513	UFT	C4'-C5'-O5'-P
1	A	545	UFT	C4'-C5'-O5'-P
1	B	545	UFT	C4'-C5'-O5'-P
1	A	593	UFT	C4'-C5'-O5'-P
1	A	684	UFT	C4'-C5'-O5'-P
1	B	684	UFT	C4'-C5'-O5'-P
1	A	49	CFZ	C3'-C4'-C5'-O5'
1	A	75	CFZ	C3'-C4'-C5'-O5'
1	A	200	UFT	O4'-C4'-C5'-O5'
1	B	200	UFT	O4'-C4'-C5'-O5'
1	A	350	UFT	C3'-C4'-C5'-O5'
1	B	352	UFT	O4'-C4'-C5'-O5'
1	A	363	CFZ	C3'-C4'-C5'-O5'
1	A	370	CFZ	C3'-C4'-C5'-O5'
1	B	370	CFZ	C3'-C4'-C5'-O5'
1	A	432	UFT	O4'-C4'-C5'-O5'
1	A	471	UFT	O4'-C4'-C5'-O5'
1	B	499	UFT	C3'-C4'-C5'-O5'
1	B	519	UFT	C3'-C4'-C5'-O5'
1	B	556	CFZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	590	UFT	O4'-C4'-C5'-O5'
1	B	609	UFT	O4'-C4'-C5'-O5'
1	B	105	UFT	C4'-C5'-O5'-P
1	B	114	CFZ	O4'-C4'-C5'-O5'
1	B	210	CFZ	O4'-C4'-C5'-O5'
1	A	332	CFZ	O4'-C4'-C5'-O5'
1	A	456	UFT	O4'-C4'-C5'-O5'
1	A	517	CFZ	O4'-C4'-C5'-O5'
1	A	542	UFT	O4'-C4'-C5'-O5'
1	B	542	UFT	O4'-C4'-C5'-O5'
1	A	556	CFZ	O4'-C4'-C5'-O5'
1	A	621	UFT	O4'-C4'-C5'-O5'
1	A	192	UFT	C4'-C5'-O5'-P
1	B	590	UFT	C4'-C5'-O5'-P
1	B	621	UFT	C4'-C5'-O5'-P
1	A	210	CFZ	O4'-C4'-C5'-O5'
1	A	432	UFT	C3'-C4'-C5'-O5'
1	B	456	UFT	O4'-C4'-C5'-O5'
1	B	473	CFZ	O4'-C4'-C5'-O5'
1	A	556	CFZ	O4'-C1'-N1-C6
1	B	50	UFT	C4'-C5'-O5'-P
1	A	196	UFT	C4'-C5'-O5'-P
1	B	229	UFT	C4'-C5'-O5'-P
1	B	360	CFZ	O4'-C4'-C5'-O5'
1	A	440	CFZ	C3'-C4'-C5'-O5'
1	B	621	UFT	O4'-C4'-C5'-O5'
1	B	667	CFZ	O4'-C4'-C5'-O5'
1	B	556	CFZ	O4'-C1'-N1-C6
1	B	10	CFZ	C4'-C5'-O5'-P
1	A	105	UFT	C4'-C5'-O5'-P
1	A	202	UFT	C4'-C5'-O5'-P
1	A	377	UFT	C4'-C5'-O5'-P
1	B	381	CFZ	C4'-C5'-O5'-P
1	B	676	UFT	C4'-C5'-O5'-P
1	B	61	UFT	C3'-C4'-C5'-O5'
1	B	74	UFT	C3'-C4'-C5'-O5'
1	A	114	CFZ	O4'-C4'-C5'-O5'
1	A	200	UFT	C3'-C4'-C5'-O5'
1	B	200	UFT	C3'-C4'-C5'-O5'
1	B	216	UFT	O4'-C4'-C5'-O5'
1	B	219	CFZ	C3'-C4'-C5'-O5'
1	B	334	UFT	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	431	UFT	C3'-C4'-C5'-O5'
1	B	431	UFT	C3'-C4'-C5'-O5'
1	B	481	UFT	C3'-C4'-C5'-O5'
1	A	499	UFT	C3'-C4'-C5'-O5'
1	A	519	UFT	C2'-C1'-N1-C2
1	B	196	UFT	C4'-C5'-O5'-P
1	B	377	UFT	C4'-C5'-O5'-P
1	B	472	UFT	C4'-C5'-O5'-P
1	A	503	UFT	C4'-C5'-O5'-P
1	A	556	CFZ	O4'-C1'-N1-C2
1	A	621	UFT	C4'-C5'-O5'-P
1	A	625	CFZ	C4'-C5'-O5'-P
1	B	625	CFZ	C4'-C5'-O5'-P
1	A	676	UFT	C4'-C5'-O5'-P
1	B	26	CFZ	O4'-C4'-C5'-O5'
1	A	28	CFZ	C3'-C4'-C5'-O5'
1	A	61	UFT	C3'-C4'-C5'-O5'
1	A	141	UFT	C3'-C4'-C5'-O5'
1	A	298	CFZ	O4'-C4'-C5'-O5'
1	B	298	CFZ	O4'-C4'-C5'-O5'
1	A	334	UFT	C3'-C4'-C5'-O5'
1	B	389	UFT	O4'-C4'-C5'-O5'
1	A	406	CFZ	O4'-C4'-C5'-O5'
1	B	406	CFZ	O4'-C4'-C5'-O5'
1	B	610	CFZ	O4'-C4'-C5'-O5'
1	A	673	UFT	C3'-C4'-C5'-O5'
1	A	708	UFT	O4'-C4'-C5'-O5'
1	B	84	UFT	C4'-C5'-O5'-P
1	B	232	CFZ	C4'-C5'-O5'-P
1	B	564	CFZ	C4'-C5'-O5'-P
1	B	593	UFT	C4'-C5'-O5'-P
1	A	666	UFT	C4'-C5'-O5'-P
1	A	94	UFT	C3'-C4'-C5'-O5'
1	A	104	CFZ	C3'-C4'-C5'-O5'
1	B	141	UFT	C3'-C4'-C5'-O5'
1	A	481	UFT	C3'-C4'-C5'-O5'
1	A	559	UFT	C3'-C4'-C5'-O5'
1	A	15	CFZ	C4'-C5'-O5'-P
1	A	84	UFT	C4'-C5'-O5'-P
1	A	564	CFZ	C4'-C5'-O5'-P
1	B	666	UFT	C4'-C5'-O5'-P
1	B	270	UFT	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	387	CFZ	O4'-C4'-C5'-O5'
1	B	440	CFZ	C3'-C4'-C5'-O5'
1	B	684	UFT	C3'-C4'-C5'-O5'
1	B	301	UFT	C3'-C4'-C5'-O5'
1	A	370	CFZ	O4'-C4'-C5'-O5'
1	B	549	UFT	C3'-C4'-C5'-O5'
1	B	673	UFT	C3'-C4'-C5'-O5'
1	B	556	CFZ	O4'-C1'-N1-C2
1	B	583	CFZ	C4'-C5'-O5'-P
1	A	28	CFZ	O4'-C4'-C5'-O5'
1	B	370	CFZ	O4'-C4'-C5'-O5'
1	A	440	CFZ	O4'-C4'-C5'-O5'
1	B	519	UFT	O4'-C4'-C5'-O5'
1	A	232	CFZ	C4'-C5'-O5'-P
1	A	344	UFT	C4'-C5'-O5'-P
1	A	583	CFZ	C4'-C5'-O5'-P
1	B	126	UFT	O4'-C4'-C5'-O5'
1	A	270	UFT	C3'-C4'-C5'-O5'
1	A	301	UFT	C3'-C4'-C5'-O5'
1	B	334	UFT	O4'-C4'-C5'-O5'
1	A	352	UFT	C3'-C4'-C5'-O5'
1	A	363	CFZ	O4'-C4'-C5'-O5'
1	B	424	CFZ	C3'-C4'-C5'-O5'
1	A	431	UFT	O4'-C4'-C5'-O5'
1	B	431	UFT	O4'-C4'-C5'-O5'
1	B	499	UFT	O4'-C4'-C5'-O5'
1	A	590	UFT	C3'-C4'-C5'-O5'
1	A	664	CFZ	O4'-C4'-C5'-O5'
1	B	664	CFZ	O4'-C4'-C5'-O5'
1	A	684	UFT	C3'-C4'-C5'-O5'
1	B	59	UFT	C3'-C4'-C5'-O5'
1	B	61	UFT	O4'-C4'-C5'-O5'
1	B	94	UFT	O4'-C4'-C5'-O5'
1	A	126	UFT	O4'-C4'-C5'-O5'
1	A	210	CFZ	C3'-C4'-C5'-O5'
1	B	210	CFZ	C3'-C4'-C5'-O5'
1	B	473	CFZ	C3'-C4'-C5'-O5'
1	B	481	UFT	O4'-C4'-C5'-O5'
1	A	556	CFZ	C3'-C4'-C5'-O5'
1	B	556	CFZ	C3'-C4'-C5'-O5'
1	A	558	CFZ	O4'-C4'-C5'-O5'
1	A	583	CFZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	B	583	CFZ	O4'-C4'-C5'-O5'
1	B	635	UFT	C3'-C4'-C5'-O5'
1	B	75	CFZ	O4'-C4'-C5'-O5'
1	A	170	UFT	C3'-C4'-C5'-O5'
1	A	352	UFT	O4'-C4'-C5'-O5'
1	A	424	CFZ	C3'-C4'-C5'-O5'
1	B	432	UFT	C3'-C4'-C5'-O5'
1	A	542	UFT	C3'-C4'-C5'-O5'
1	B	549	UFT	O4'-C4'-C5'-O5'
1	A	635	UFT	C3'-C4'-C5'-O5'
1	A	673	UFT	O4'-C4'-C5'-O5'
1	A	101	UFT	C4'-C5'-O5'-P
1	A	50	UFT	C3'-C4'-C5'-O5'
1	A	61	UFT	O4'-C4'-C5'-O5'
1	B	170	UFT	C3'-C4'-C5'-O5'
1	A	321	CFZ	O4'-C4'-C5'-O5'
1	B	360	CFZ	C3'-C4'-C5'-O5'
1	B	489	UFT	O4'-C4'-C5'-O5'
1	A	499	UFT	O4'-C4'-C5'-O5'
1	B	523	CFZ	O4'-C4'-C5'-O5'
1	B	542	UFT	C3'-C4'-C5'-O5'
1	A	548	CFZ	C3'-C4'-C5'-O5'
1	A	472	UFT	C4'-C5'-O5'-P
1	B	219	CFZ	O4'-C4'-C5'-O5'
1	A	334	UFT	O4'-C4'-C5'-O5'
1	A	381	CFZ	C4'-C5'-O5'-P
1	B	555	UFT	C4'-C5'-O5'-P
1	A	513	UFT	C3'-C4'-C5'-O5'

There are no ring outliers.

294 monomers are involved in 386 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	200	UFT	1	0
1	B	446	CFZ	1	0
1	B	402	UFT	1	0
1	B	695	UFT	1	0
1	B	328	CFZ	2	0
1	B	458	CFZ	1	0
1	A	372	CFZ	1	0
1	A	10	CFZ	1	0
1	A	322	UFT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	477	CFZ	1	0
1	A	643	CFZ	1	0
1	A	233	UFT	1	0
1	B	372	CFZ	2	0
1	B	509	UFT	2	0
1	B	558	CFZ	1	0
1	B	219	CFZ	2	0
1	A	548	CFZ	1	0
1	A	513	UFT	1	0
1	B	293	UFT	1	0
1	B	549	UFT	2	0
1	B	719	UFT	3	0
1	A	215	UFT	1	0
1	B	210	CFZ	1	0
1	A	417	CFZ	1	0
1	B	411	CFZ	2	0
1	B	485	UFT	1	0
1	A	347	UFT	1	0
1	A	366	UFT	1	0
1	B	94	UFT	1	0
1	B	556	CFZ	2	0
1	B	365	UFT	1	0
1	A	316	CFZ	2	0
1	A	79	CFZ	2	0
1	A	165	CFZ	3	0
1	A	695	UFT	1	0
1	B	21	CFZ	3	0
1	A	633	UFT	2	0
1	A	21	CFZ	2	0
1	A	355	CFZ	3	0
1	A	387	CFZ	1	0
1	B	628	UFT	1	0
1	B	498	CFZ	1	0
1	B	489	UFT	1	0
1	B	518	CFZ	1	0
1	B	246	CFZ	2	0
1	B	25	CFZ	1	0
1	B	154	UFT	1	0
1	B	602	UFT	2	0
1	A	169	UFT	1	0
1	A	103	CFZ	1	0
1	B	106	UFT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	153	UFT	1	0
1	B	637	CFZ	1	0
1	B	184	CFZ	1	0
1	A	609	UFT	1	0
1	A	669	UFT	2	0
1	A	216	UFT	1	0
1	A	84	UFT	1	0
1	B	571	UFT	1	0
1	B	80	UFT	2	0
1	A	96	CFZ	1	0
1	B	472	UFT	2	0
1	B	84	UFT	1	0
1	A	600	CFZ	2	0
1	A	214	UFT	1	0
1	B	555	UFT	1	0
1	B	418	CFZ	2	0
1	B	698	CFZ	3	0
1	A	486	CFZ	1	0
1	B	362	CFZ	1	0
1	A	265	UFT	1	0
1	A	204	UFT	1	0
1	A	430	UFT	2	0
1	B	535	UFT	1	0
1	B	647	CFZ	1	0
1	A	518	CFZ	1	0
1	A	179	UFT	2	0
1	A	33	UFT	2	0
1	B	218	CFZ	2	0
1	B	156	CFZ	1	0
1	A	551	CFZ	2	0
1	B	71	UFT	1	0
1	A	471	UFT	1	0
1	A	14	UFT	1	0
1	A	481	UFT	1	0
1	A	323	CFZ	1	0
1	B	687	UFT	2	0
1	A	315	CFZ	1	0
1	A	673	UFT	1	0
1	A	140	CFZ	1	0
1	B	437	UFT	1	0
1	B	629	UFT	3	0
1	A	313	UFT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	350	UFT	1	0
1	A	425	CFZ	1	0
1	B	120	CFZ	2	0
1	A	359	UFT	1	0
1	A	549	UFT	4	0
1	A	57	CFZ	1	0
1	B	492	CFZ	5	0
1	A	693	CFZ	2	0
1	B	669	UFT	2	0
1	A	112	UFT	2	0
1	B	179	UFT	2	0
1	B	338	CFZ	1	0
1	B	279	CFZ	3	0
1	A	171	CFZ	1	0
1	A	260	UFT	3	0
1	A	637	CFZ	1	0
1	B	169	UFT	1	0
1	B	600	CFZ	2	0
1	B	140	CFZ	1	0
1	A	517	CFZ	1	0
1	B	197	UFT	1	0
1	B	135	UFT	5	0
1	B	74	UFT	1	0
1	A	418	CFZ	2	0
1	B	316	CFZ	2	0
1	A	492	CFZ	1	0
1	B	389	UFT	2	0
1	A	156	CFZ	1	0
1	A	498	CFZ	2	0
1	B	423	UFT	1	0
1	B	633	UFT	2	0
1	A	459	CFZ	1	0
1	B	511	CFZ	2	0
1	A	105	UFT	1	0
1	A	351	CFZ	2	0
1	B	421	UFT	1	0
1	A	687	UFT	2	0
1	A	444	CFZ	1	0
1	A	629	UFT	3	0
1	B	214	UFT	1	0
1	B	464	UFT	1	0
1	B	315	CFZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	402	UFT	1	0
1	B	491	CFZ	3	0
1	B	673	UFT	1	0
1	A	446	CFZ	1	0
1	B	424	CFZ	1	0
1	B	592	CFZ	1	0
1	B	512	CFZ	1	0
1	B	209	CFZ	4	0
1	A	208	UFT	2	0
1	B	32	UFT	2	0
1	B	33	UFT	2	0
1	A	234	CFZ	1	0
1	A	32	UFT	1	0
1	B	459	CFZ	1	0
1	A	108	UFT	1	0
1	A	646	UFT	2	0
1	B	430	UFT	1	0
1	B	247	CFZ	4	0
1	A	344	UFT	2	0
1	B	471	UFT	1	0
1	B	481	UFT	1	0
1	A	659	UFT	1	0
1	B	631	CFZ	1	0
1	A	217	UFT	3	0
1	B	234	CFZ	2	0
1	B	536	CFZ	1	0
1	A	647	CFZ	1	0
1	B	587	CFZ	1	0
1	A	73	CFZ	1	0
1	B	366	UFT	1	0
1	B	55	UFT	3	0
1	A	120	CFZ	2	0
1	A	293	UFT	1	0
1	B	441	CFZ	2	0
1	A	328	CFZ	2	0
1	A	628	UFT	1	0
1	A	137	UFT	2	0
1	B	548	CFZ	1	0
1	B	282	CFZ	1	0
1	A	11	UFT	3	0
1	B	593	UFT	1	0
1	B	712	UFT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	432	UFT	1	0
1	A	365	UFT	2	0
1	A	43	UFT	1	0
1	B	493	UFT	3	0
1	A	210	CFZ	1	0
1	A	184	CFZ	1	0
1	A	436	CFZ	1	0
1	B	577	UFT	2	0
1	A	411	CFZ	3	0
1	B	708	UFT	1	0
1	A	472	UFT	2	0
1	A	279	CFZ	3	0
1	A	242	CFZ	1	0
1	A	556	CFZ	3	0
1	A	336	UFT	1	0
1	B	171	CFZ	1	0
1	A	698	CFZ	3	0
1	A	59	UFT	1	0
1	B	432	UFT	1	0
1	A	197	UFT	1	0
1	B	363	CFZ	1	0
1	B	425	CFZ	1	0
1	B	351	CFZ	1	0
1	B	265	UFT	1	0
1	A	218	CFZ	2	0
1	B	646	UFT	2	0
1	B	34	CFZ	1	0
1	A	602	UFT	2	0
1	B	693	CFZ	2	0
1	A	60	UFT	1	0
1	A	464	UFT	1	0
1	A	72	CFZ	1	0
1	B	233	UFT	2	0
1	A	149	CFZ	1	0
1	B	165	CFZ	2	0
1	A	354	CFZ	2	0
1	A	571	UFT	1	0
1	B	465	CFZ	1	0
1	A	154	UFT	1	0
1	A	610	CFZ	1	0
1	B	323	CFZ	2	0
1	B	513	UFT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	577	UFT	2	0
1	B	659	UFT	1	0
1	B	96	CFZ	1	0
1	A	512	CFZ	1	0
1	B	519	UFT	1	0
1	A	106	UFT	1	0
1	A	437	UFT	1	0
1	B	260	UFT	4	0
1	A	558	CFZ	1	0
1	B	208	UFT	2	0
1	A	424	CFZ	1	0
1	A	423	UFT	1	0
1	B	460	UFT	1	0
1	B	517	CFZ	1	0
1	A	249	CFZ	1	0
1	B	149	CFZ	1	0
1	A	550	CFZ	2	0
1	B	550	CFZ	3	0
1	B	216	UFT	1	0
1	B	403	UFT	1	0
1	A	80	UFT	3	0
1	B	112	UFT	2	0
1	A	34	CFZ	1	0
1	B	551	CFZ	4	0
1	A	509	UFT	2	0
1	A	477	CFZ	1	0
1	A	535	UFT	1	0
1	B	8	UFT	1	0
1	B	28	CFZ	2	0
1	A	574	CFZ	1	0
1	B	720	UFT	4	0
1	A	209	CFZ	4	0
1	A	708	UFT	1	0
1	A	441	CFZ	2	0
1	B	494	CFZ	2	0
1	A	590	UFT	2	0
1	A	164	CFZ	1	0
1	A	139	CFZ	1	0
1	A	519	UFT	3	0
1	A	511	CFZ	3	0
1	A	720	UFT	1	0
1	B	10	CFZ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	421	UFT	1	0
1	B	13	UFT	1	0
1	A	465	CFZ	1	0
1	A	460	UFT	1	0
1	B	620	CFZ	1	0
1	B	679	CFZ	1	0
1	A	135	UFT	4	0
1	B	14	UFT	1	0
1	B	217	UFT	3	0
1	B	92	UFT	1	0
1	B	215	UFT	1	0
1	A	403	UFT	1	0
1	A	254	CFZ	1	0
1	A	71	UFT	1	0
1	B	417	CFZ	2	0
1	B	204	UFT	2	0
1	A	413	UFT	1	0
1	B	139	CFZ	1	0
1	A	631	CFZ	1	0
1	A	458	CFZ	2	0
1	A	144	CFZ	1	0
1	B	157	CFZ	3	0
1	B	105	UFT	1	0
1	A	593	UFT	1	0
1	A	157	CFZ	3	0
1	B	137	UFT	2	0
1	A	153	UFT	1	0
1	A	55	UFT	2	0
1	A	247	CFZ	1	0
1	B	643	CFZ	1	0
1	B	173	CFZ	1	0
1	A	173	CFZ	1	0
1	B	486	CFZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54779. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

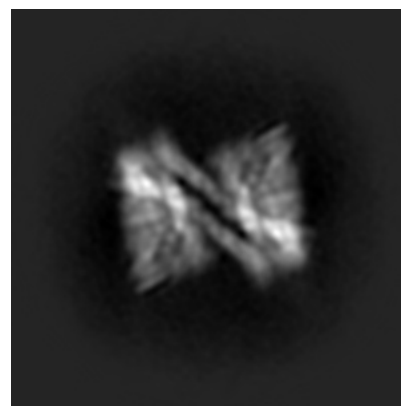
6.1.1 Primary map



X

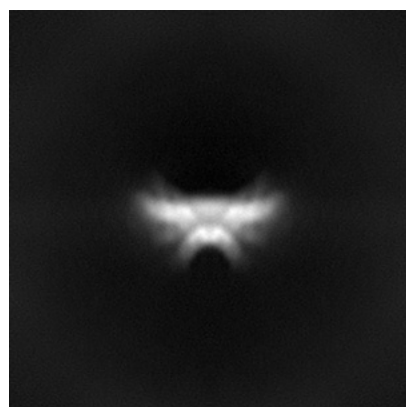


Y

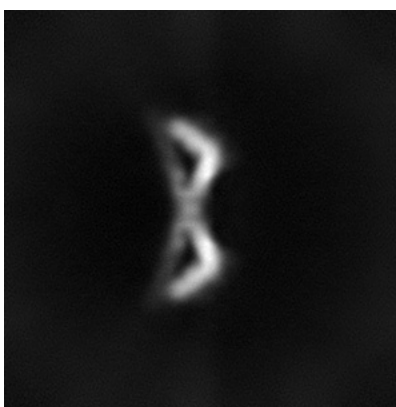


Z

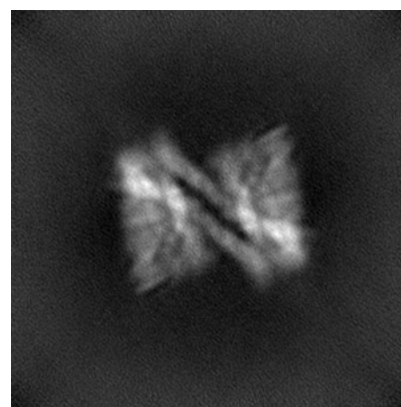
6.1.2 Raw map



X



Y

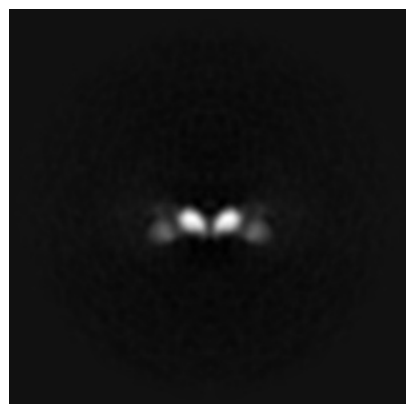


Z

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

6.2 Central slices [i](#)

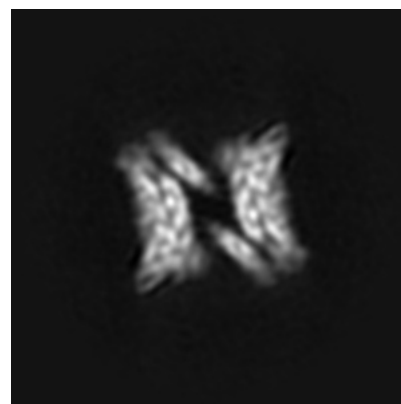
6.2.1 Primary map



X Index: 128

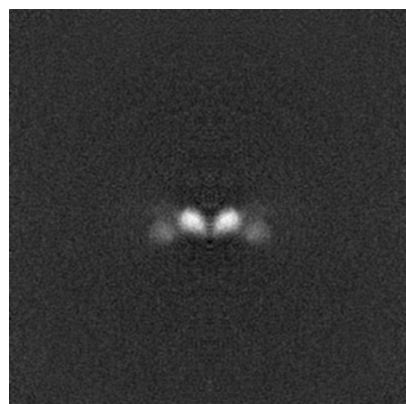


Y Index: 128

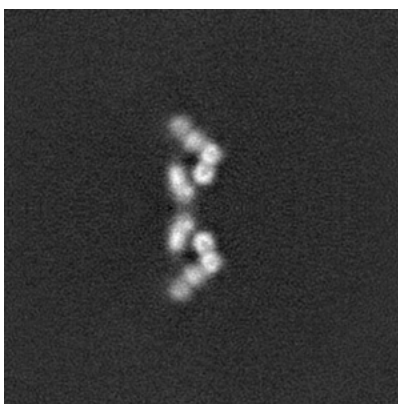


Z Index: 128

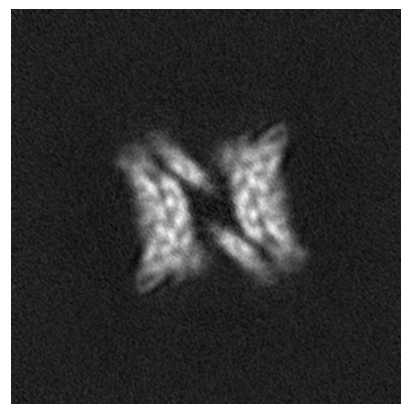
6.2.2 Raw map



X Index: 128



Y Index: 128

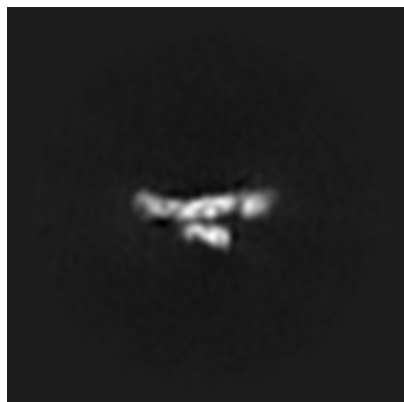


Z Index: 128

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

6.3 Largest variance slices [i](#)

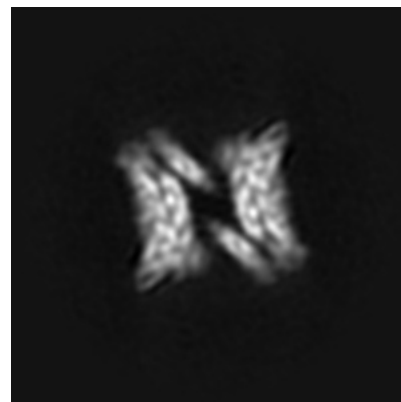
6.3.1 Primary map



X Index: 106



Y Index: 124



Z Index: 128

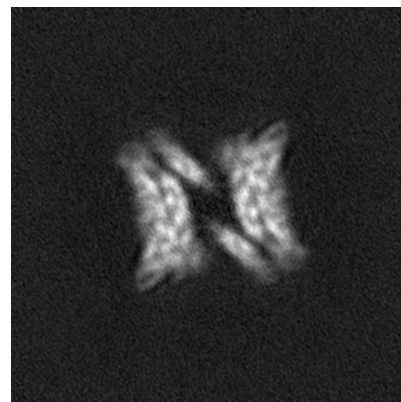
6.3.2 Raw map



X Index: 105



Y Index: 125



Z Index: 128

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

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

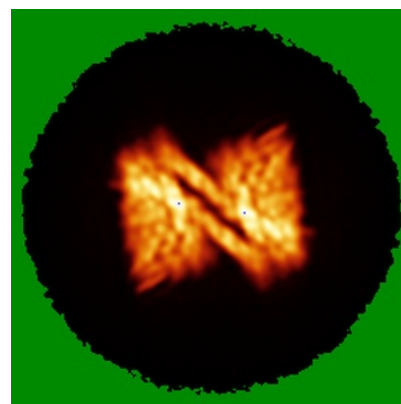
6.4.1 Primary map



X



Y

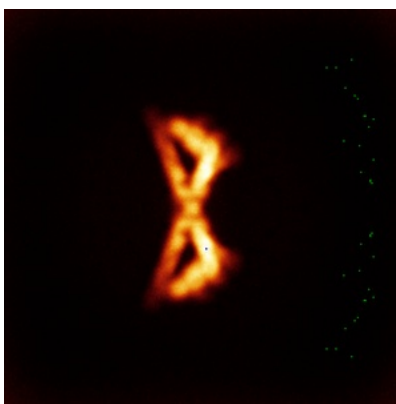


Z

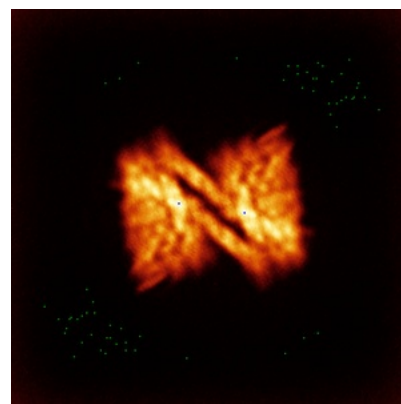
6.4.2 Raw map



X



Y

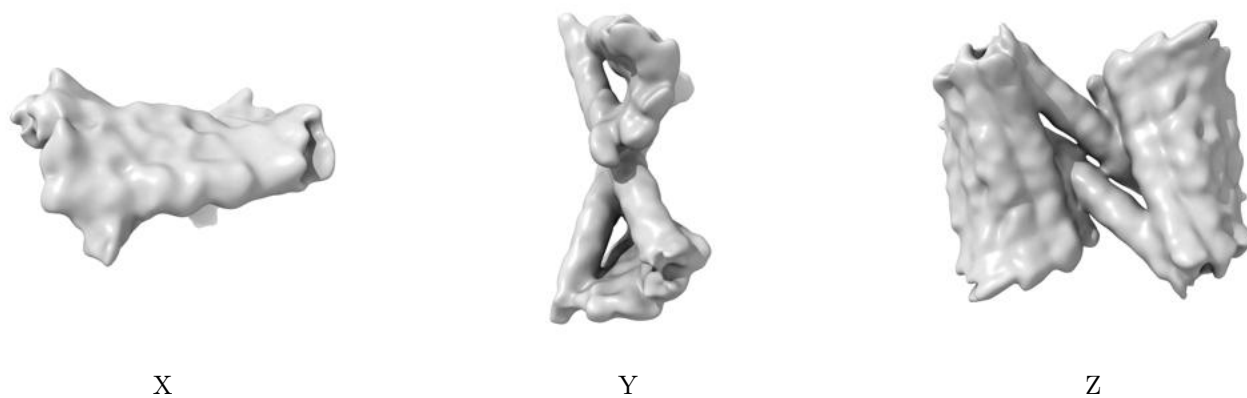


Z

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

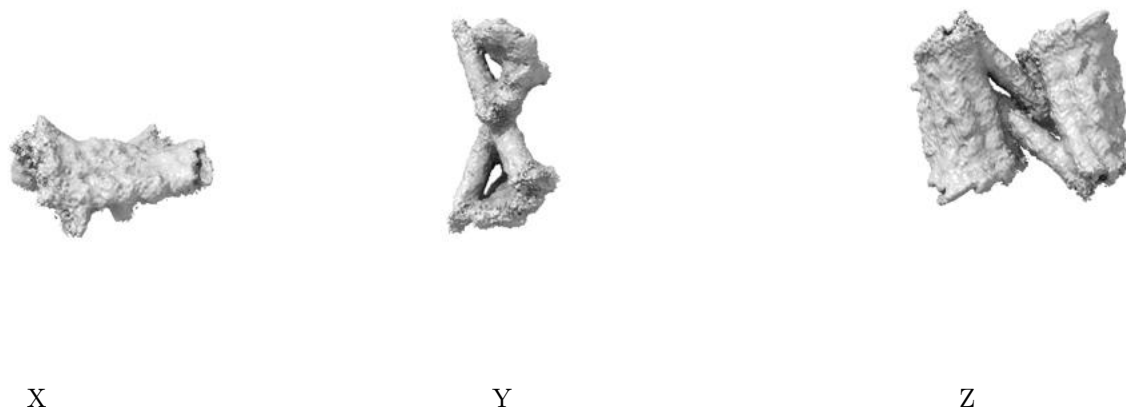
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.128. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

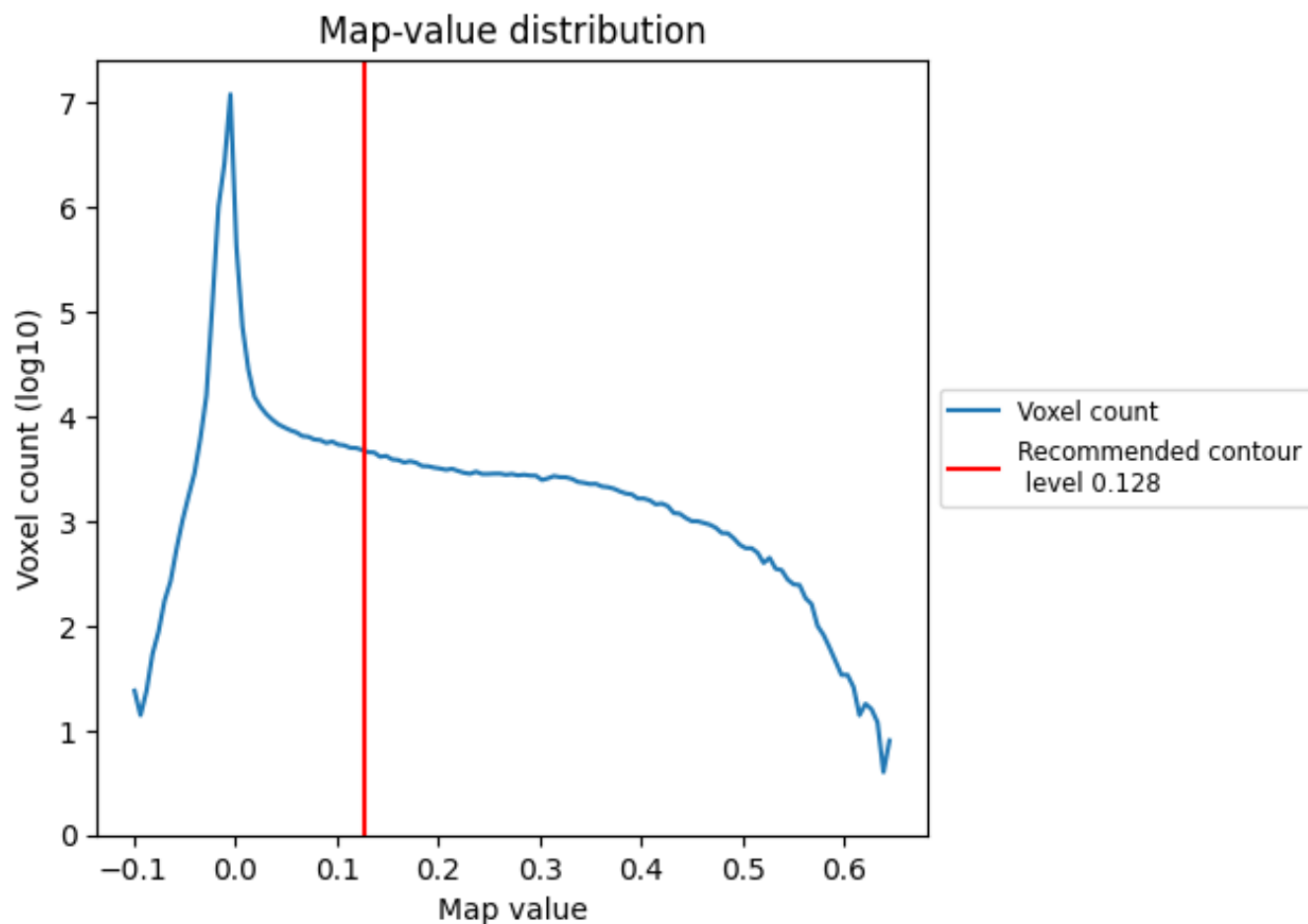
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

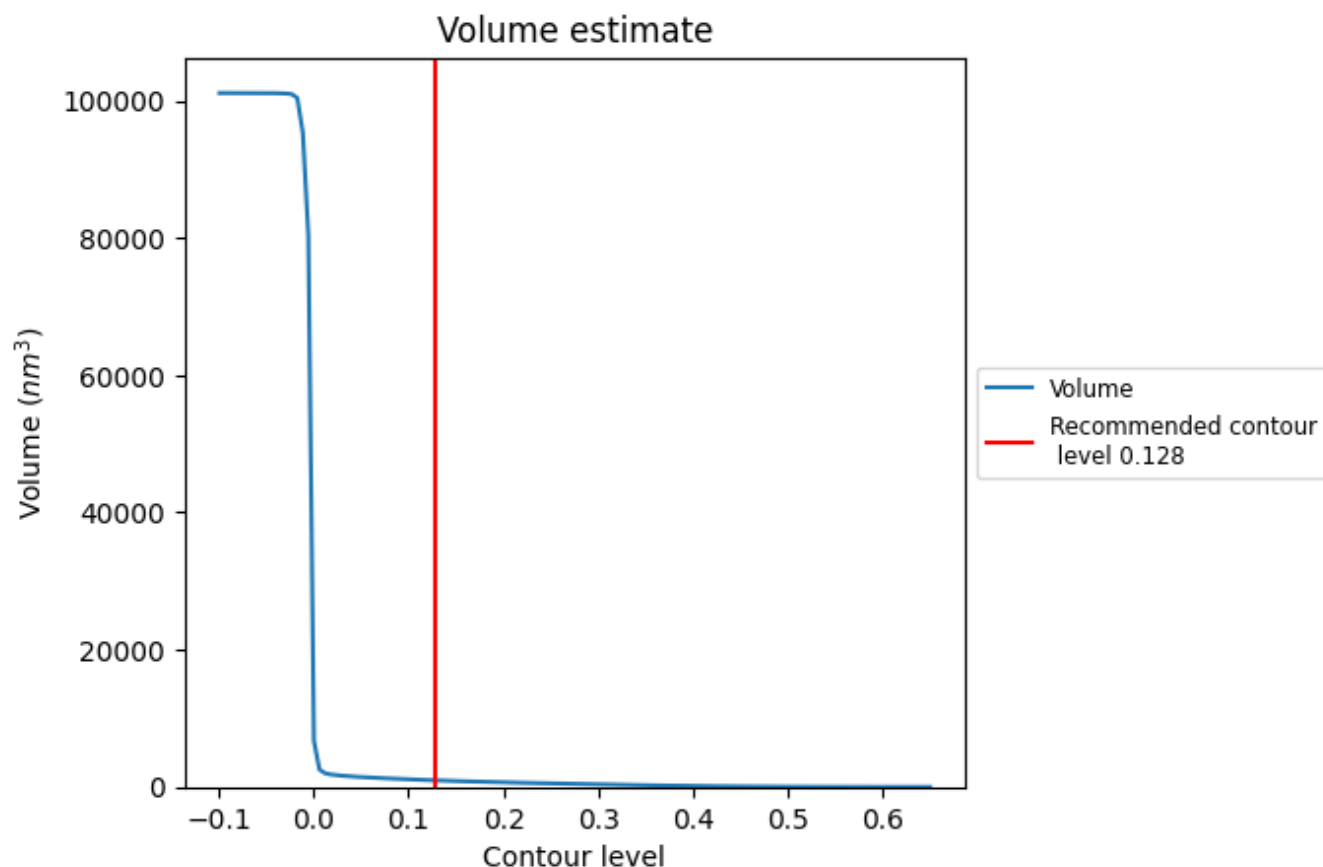
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

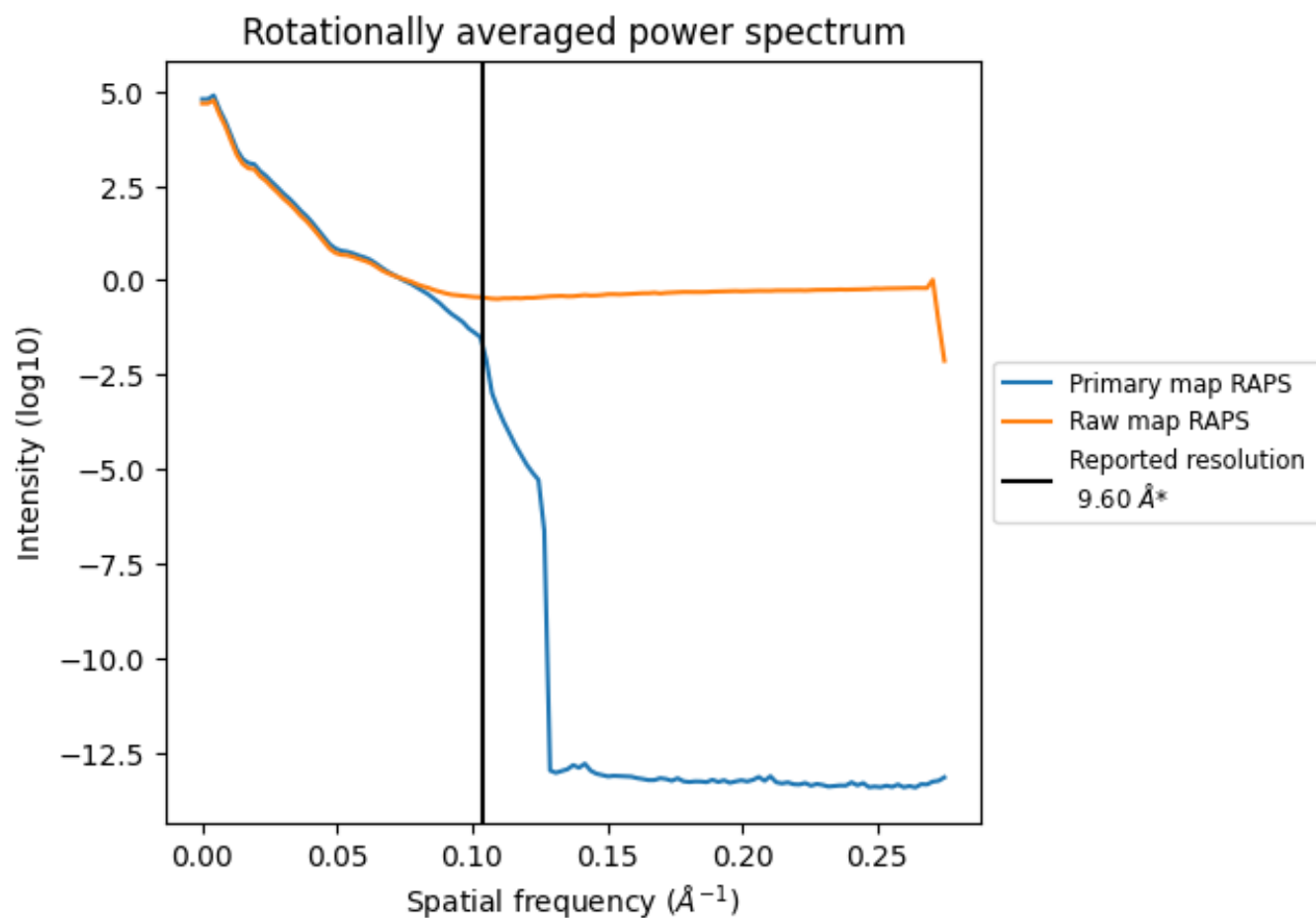
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 963 nm^3 ; this corresponds to an approximate mass of 870 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

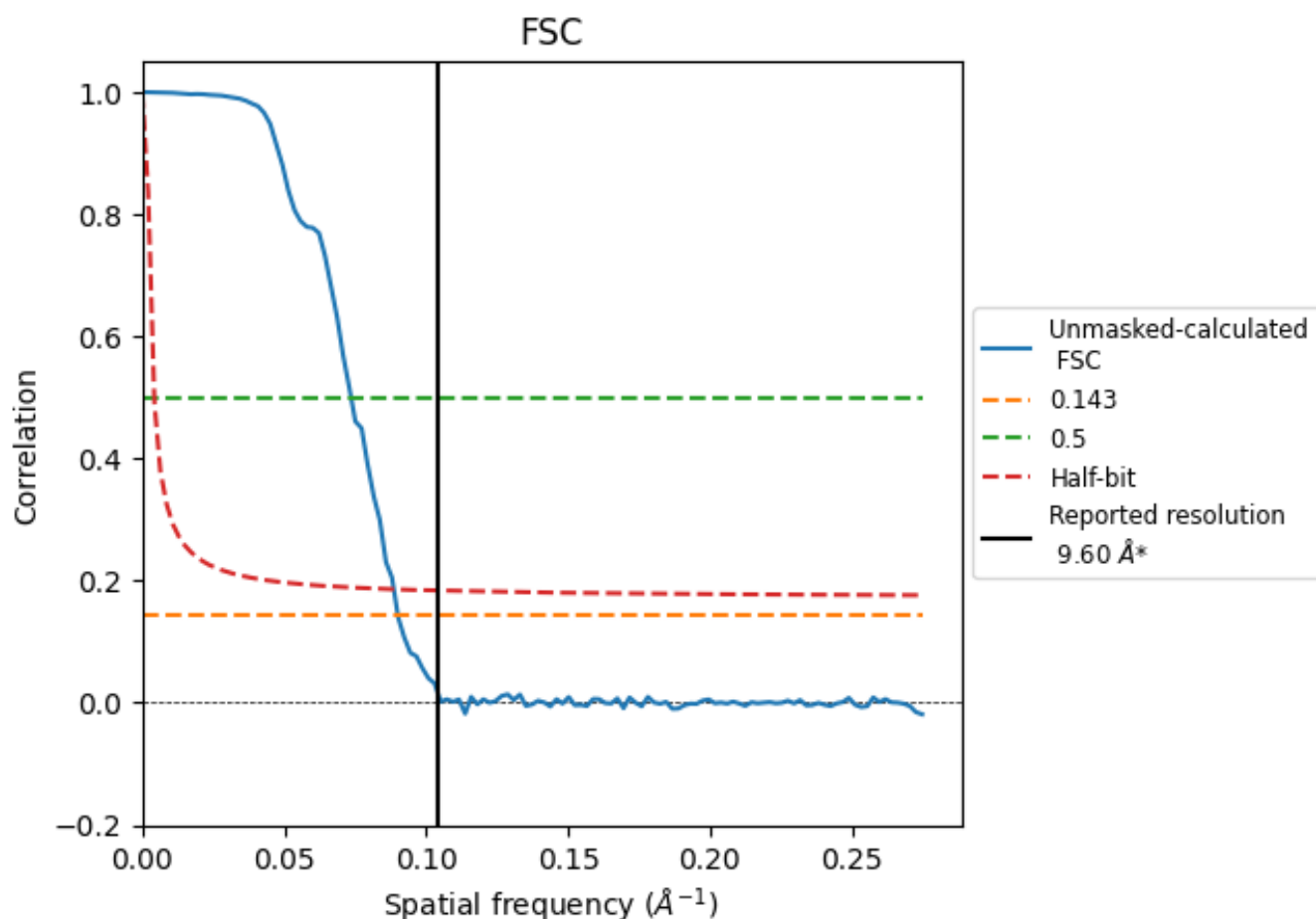


*Reported resolution corresponds to spatial frequency of 0.104 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.104 \AA^{-1}

8.2 Resolution estimates [i](#)

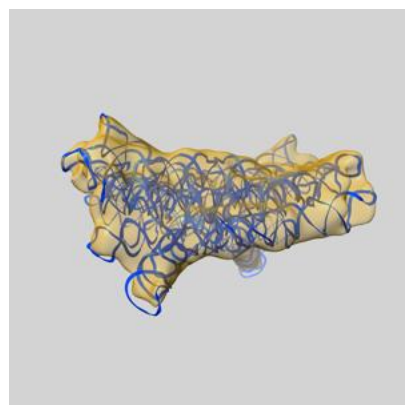
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	11.11	13.59	11.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 11.11 differs from the reported value 9.6 by more than 10 %

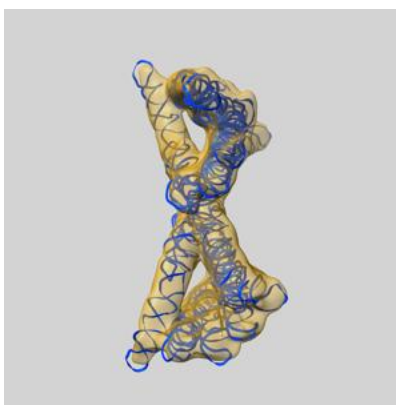
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54779 and PDB model 9SD9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

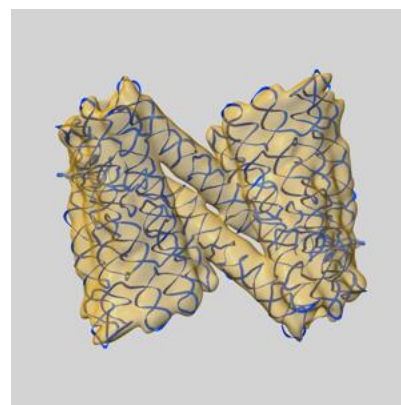
9.1 Map-model overlay [i](#)



X



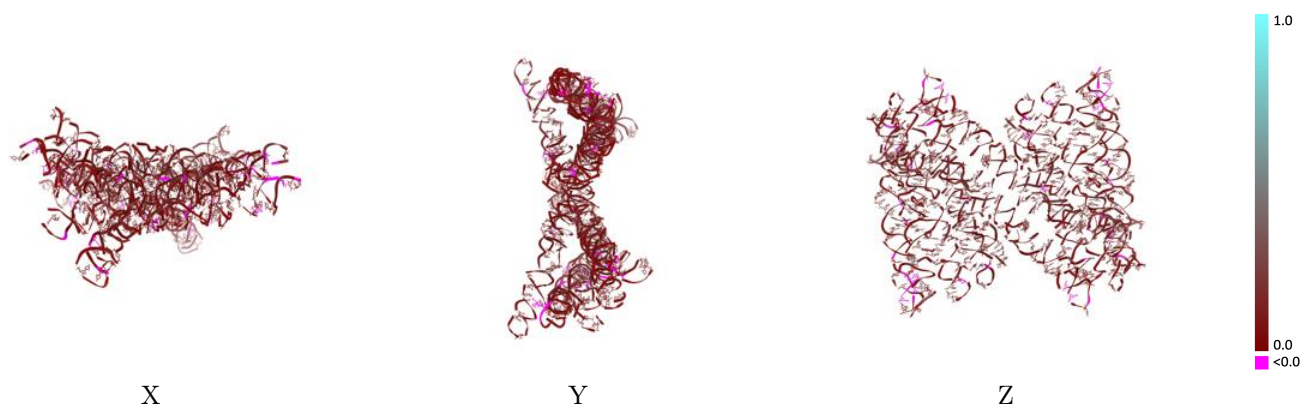
Y



Z

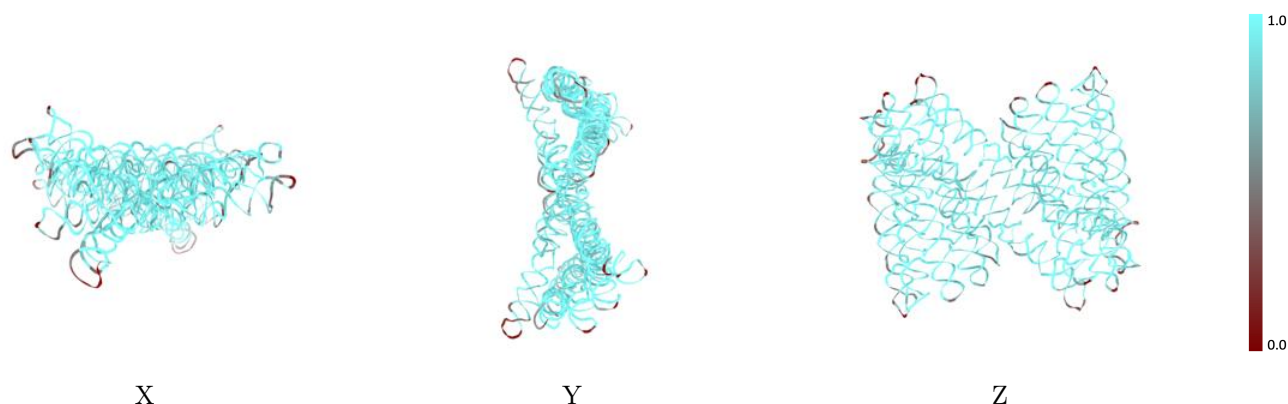
The images above show the 3D surface view of the map at the recommended contour level 0.128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



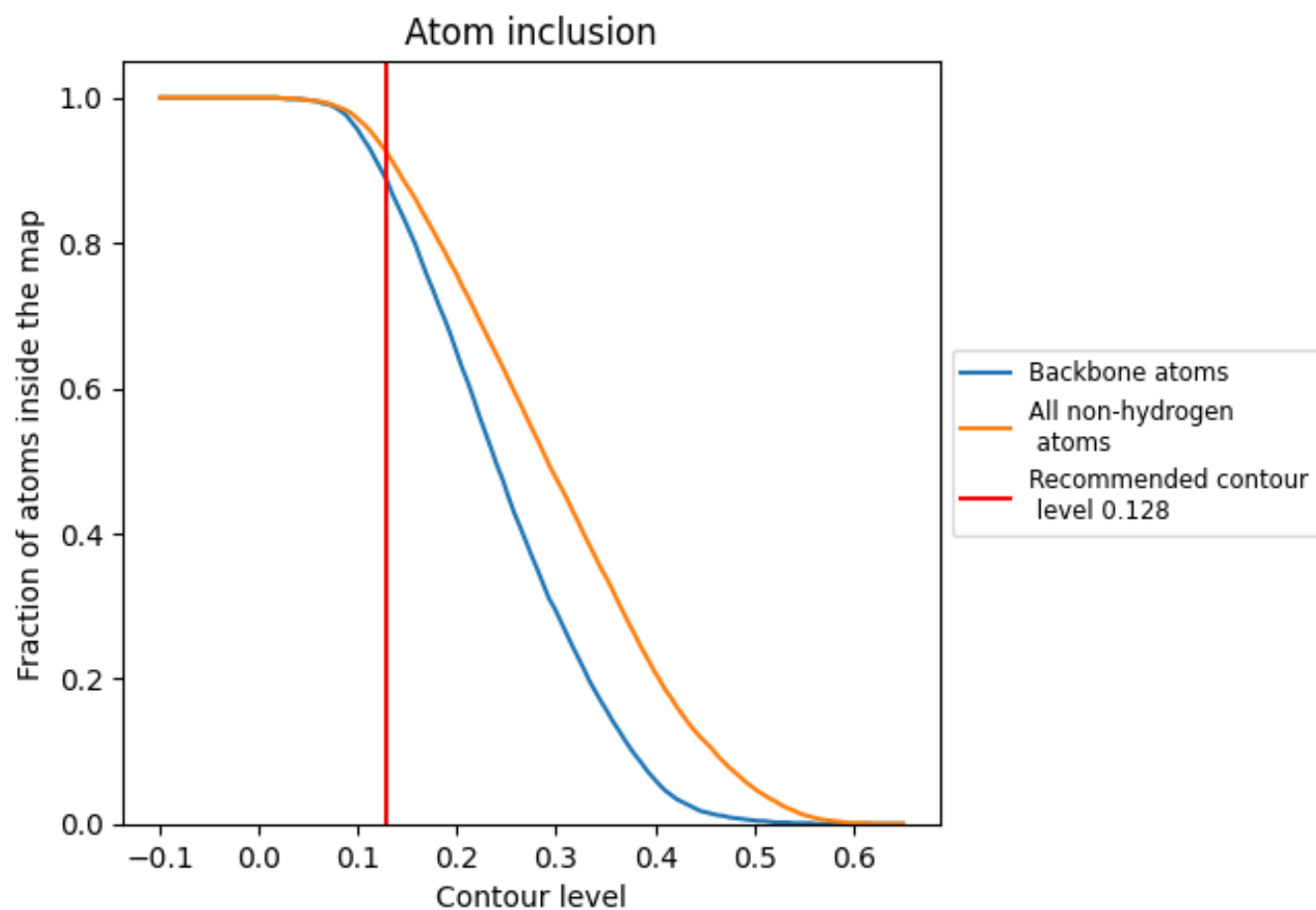
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.128).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9270	<div></div> 0.0950
A	<div></div> 0.9260	<div></div> 0.0940
B	<div></div> 0.9280	<div></div> 0.0950

