



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:26 AM UTC

PDB ID : 9R82 / pdb\_00009r82  
EMDB ID : EMD-53803  
Title : 6-Helix Bundle - with a Clasp (6HB-C)-monomer with 2'-Fluoro-modified pyrimidines (FY RNA)  
Authors : Kristoffersen, E.L.; Andersen, E.S.; Zwergius, N.H.  
Deposited on : 2025-05-15  
Resolution : 9.33 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](mailto: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>.

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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 : 2022.3.0, CSD as543be (2022)  
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



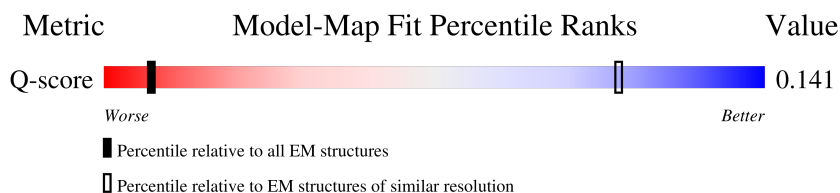
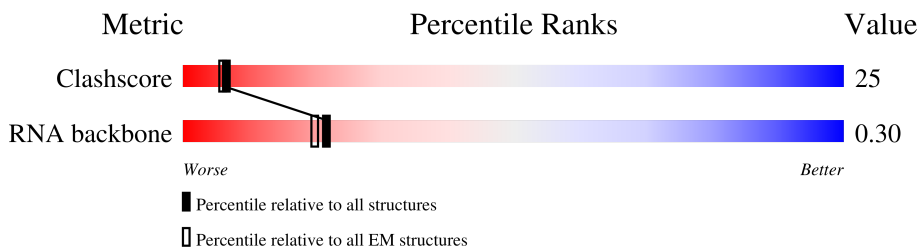
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.33 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	215 ( 8.90 - 9.83 )

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  $\geq 3$ , 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	728	



## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15523 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 DNA/RNA (728-MER).

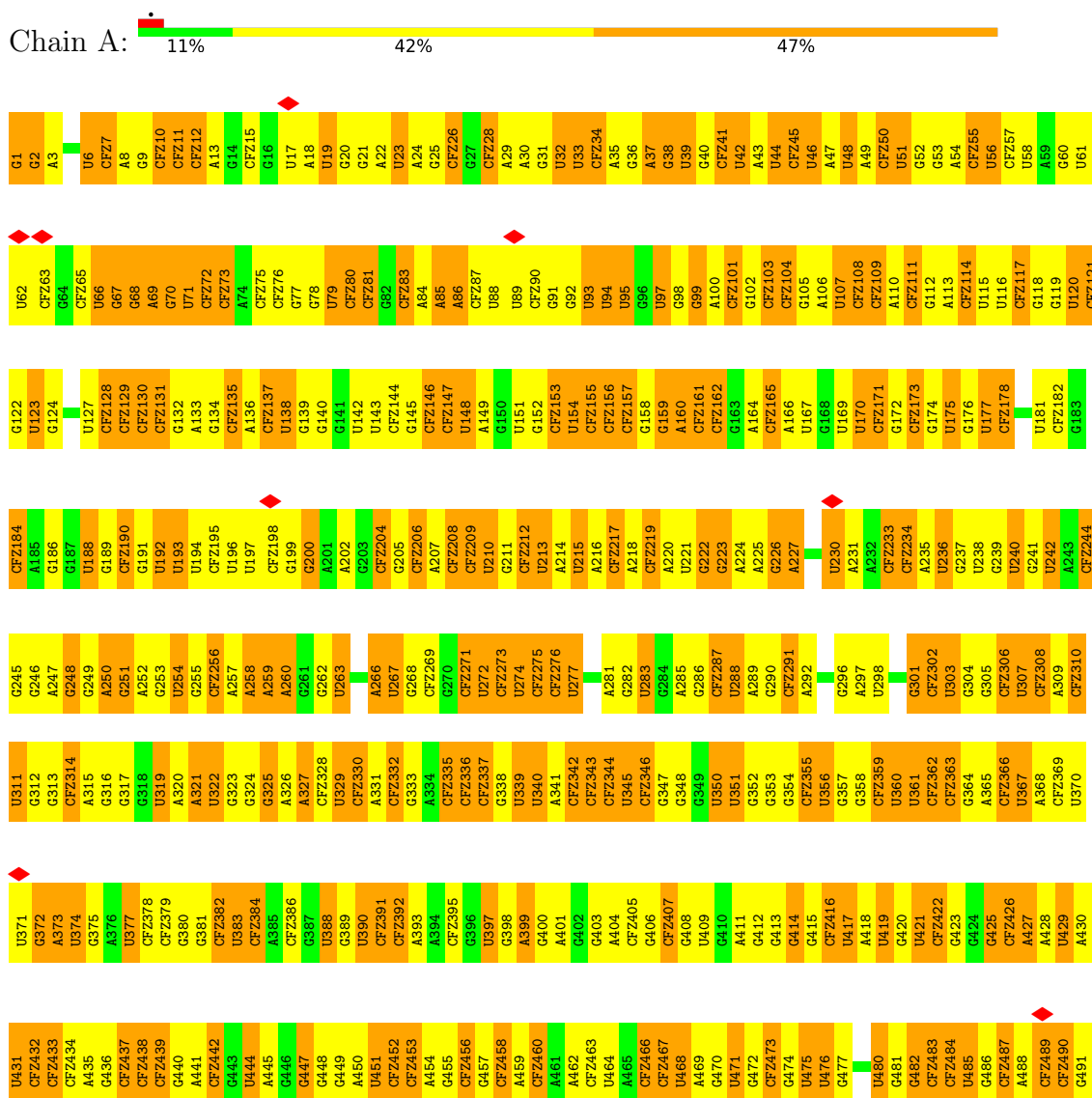
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	F	N	O	P		
1	A	728	15523	6919	361	2758	4757	728	0	0



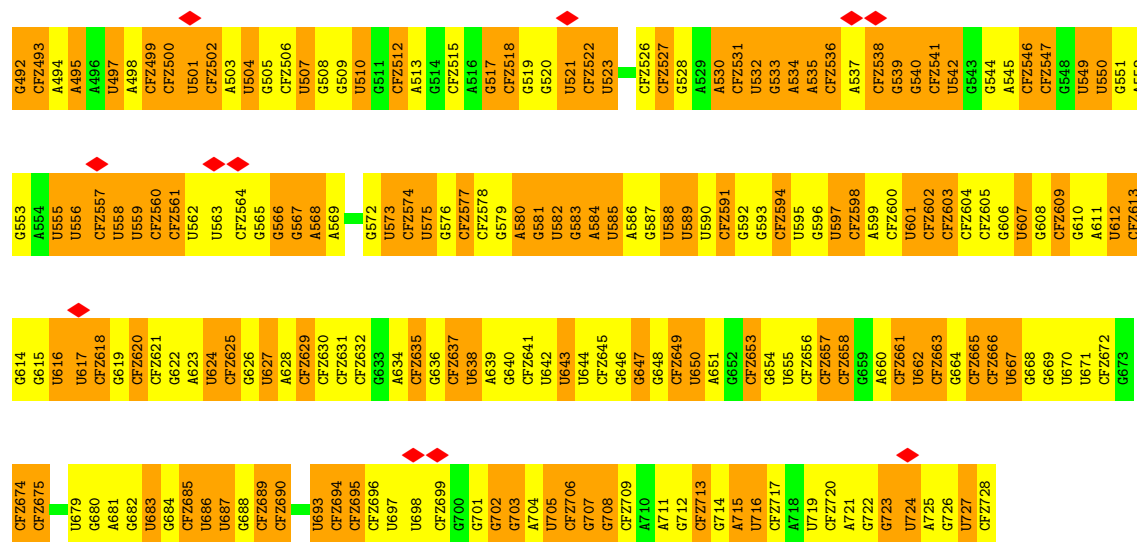
### 3 Residue-property plots

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: DNA/RNA (728-MER)









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11445	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	0.416	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	331.264, 331.264, 331.264	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.294, 1.294, 1.294	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	0.51	44/9303 (0.5%)	0.39	0/14367

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	UFT	O3'-P	6.75	1.63	1.56
1	A	497	UFT	O3'-P	6.62	1.62	1.56
1	A	322	UFT	O3'-P	6.38	1.62	1.56
1	A	66	UFT	O3'-P	6.36	1.62	1.56
1	A	17	UFT	O3'-P	6.30	1.62	1.56
1	A	471	UFT	O3'-P	5.98	1.62	1.56
1	A	340	UFT	O3'-P	5.94	1.62	1.56
1	A	242	UFT	O3'-P	5.89	1.62	1.56
1	A	504	UFT	O3'-P	5.89	1.62	1.56
1	A	429	UFT	O3'-P	5.81	1.62	1.56
1	A	288	UFT	O3'-P	5.79	1.62	1.56
1	A	23	UFT	O3'-P	5.76	1.62	1.56
1	A	607	UFT	O3'-P	5.75	1.61	1.56
1	A	679	UFT	O3'-P	5.70	1.61	1.56
1	A	97	UFT	O3'-P	5.69	1.61	1.56
1	A	267	UFT	O3'-P	5.67	1.61	1.56
1	A	417	UFT	O3'-P	5.64	1.61	1.56
1	A	48	UFT	O3'-P	5.63	1.61	1.56
1	A	371	UFT	O3'-P	5.46	1.61	1.56
1	A	213	UFT	O3'-P	5.45	1.61	1.56
1	A	585	UFT	O3'-P	5.43	1.61	1.56
1	A	510	UFT	O3'-P	5.42	1.61	1.56
1	A	254	UFT	O3'-P	5.40	1.61	1.56
1	A	464	UFT	O3'-P	5.37	1.61	1.56
1	A	582	UFT	O3'-P	5.37	1.61	1.56
1	A	210	UFT	O3'-P	5.34	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	UFT	O3'-P	5.33	1.61	1.56
1	A	683	UFT	O3'-P	5.31	1.61	1.56
1	A	58	UFT	O3'-P	5.31	1.61	1.56
1	A	148	UFT	O3'-P	5.30	1.61	1.56
1	A	42	UFT	O3'-P	5.28	1.61	1.56
1	A	138	UFT	O3'-P	5.27	1.61	1.56
1	A	263	UFT	O3'-P	5.25	1.61	1.56
1	A	367	UFT	O3'-P	5.25	1.61	1.56
1	A	19	UFT	O3'-P	5.24	1.61	1.56
1	A	188	UFT	O3'-P	5.22	1.61	1.56
1	A	230	UFT	O3'-P	5.22	1.61	1.56
1	A	687	UFT	O3'-P	5.19	1.61	1.56
1	A	351	UFT	O3'-P	5.16	1.61	1.56
1	A	476	UFT	O3'-P	5.16	1.61	1.56
1	A	627	UFT	O3'-P	5.15	1.61	1.56
1	A	419	UFT	O3'-P	5.14	1.61	1.56
1	A	277	UFT	O3'-P	5.11	1.61	1.56
1	A	221	UFT	O3'-P	5.00	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

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	15523	0	7488	574	0
All	All	15523	0	7488	574	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 25.

All (574) 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:377:UFT:HN3	1:A:715:A:N6	1.43	1.16
1:A:377:UFT:O4	1:A:715:A:N1	1.97	0.97
1:A:260:A:N6	1:A:468:UFT:HN3	1.64	0.95
1:A:377:UFT:HN3	1:A:715:A:H61	0.95	0.93
1:A:29:A:H61	1:A:37:A:N6	1.69	0.89
1:A:459:A:H61	1:A:471:UFT:HN3	1.19	0.88
1:A:260:A:H61	1:A:468:UFT:HN3	0.87	0.86
1:A:283:UFT:HN3	1:A:309:A:H61	1.26	0.84
1:A:222:G:H1	1:A:234:CFZ:HN4	1.28	0.79
1:A:607:UFT:O2	1:A:629:CFZ:N4	2.16	0.79
1:A:337:CFZ:H2'	1:A:338:G:H8	1.49	0.78
1:A:415:G:H2'	1:A:416:CFZ:H6	1.66	0.77
1:A:438:CFZ:H2'	1:A:439:CFZ:H6	1.67	0.76
1:A:665:CFZ:H2'	1:A:666:CFZ:H6	1.67	0.75
1:A:39:UFT:H2'	1:A:40:G:H8	1.52	0.75
1:A:258:A:H61	1:A:266:A:H61	1.35	0.75
1:A:92:G:H2'	1:A:93:UFT:H6	1.69	0.74
1:A:315:A:H61	1:A:345:UFT:HN3	1.35	0.74
1:A:377:UFT:N3	1:A:715:A:N6	2.19	0.74
1:A:29:A:H61	1:A:37:A:H61	1.32	0.74
1:A:217:CFZ:HN4	1:A:239:G:H1	1.35	0.74
1:A:103:CFZ:H2'	1:A:104:CFZ:H6	1.70	0.74
1:A:107:UFT:H2'	1:A:108:CFZ:H6	1.70	0.74
1:A:611:A:H2'	1:A:612:UFT:H6	1.71	0.72
1:A:46:UFT:H2'	1:A:47:A:H8	1.55	0.72
1:A:41:CFZ:H2'	1:A:42:UFT:H6	1.72	0.72
1:A:29:A:N6	1:A:37:A:H61	1.86	0.72
1:A:579:G:H2'	1:A:580:A:H8	1.55	0.71
1:A:355:CFZ:H2'	1:A:356:UFT:H6	1.73	0.71
1:A:177:UFT:H2'	1:A:178:CFZ:H6	1.73	0.70
1:A:541:CFZ:H2'	1:A:542:UFT:H6	1.73	0.70
1:A:148:UFT:H2'	1:A:149:A:H8	1.56	0.70
1:A:273:CFZ:H2'	1:A:274:UFT:H6	1.74	0.70
1:A:609:CFZ:H2'	1:A:610:G:H8	1.57	0.69
1:A:340:UFT:H2'	1:A:341:A:H8	1.57	0.69
1:A:189:G:H2'	1:A:190:CFZ:H6	1.74	0.69
1:A:643:UFT:H2'	1:A:646:G:H22	1.56	0.69
1:A:592:G:H2'	1:A:593:G:C8	2.28	0.69
1:A:649:CFZ:H2'	1:A:650:UFT:H6	1.75	0.69
1:A:484:CFZ:H2'	1:A:485:UFT:H6	1.74	0.69
1:A:350:UFT:H2'	1:A:351:UFT:H6	1.74	0.68
1:A:97:UFT:H2'	1:A:98:G:C8	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:CFZ:H2'	1:A:417:UFT:H6	1.75	0.68
1:A:555:UFT:H2'	1:A:556:UFT:H6	1.76	0.68
1:A:552:A:H2'	1:A:553:G:H8	1.59	0.68
1:A:190:CFZ:H2'	1:A:191:G:H8	1.58	0.68
1:A:257:A:H3'	1:A:258:A:H2'	1.76	0.68
1:A:40:G:H2'	1:A:41:CFZ:H6	1.74	0.68
1:A:375:G:OP1	1:A:375:G:H4'	1.92	0.67
1:A:549:UFT:H2'	1:A:550:UFT:H6	1.76	0.67
1:A:607:UFT:N3	1:A:608:G:N7	2.43	0.67
1:A:449:G:H2'	1:A:450:A:H8	1.59	0.67
1:A:414:G:H2'	1:A:415:G:H8	1.60	0.67
1:A:418:A:H2'	1:A:419:UFT:H6	1.75	0.67
1:A:148:UFT:H2'	1:A:149:A:C8	2.29	0.66
1:A:188:UFT:HN3	1:A:207:A:H61	1.39	0.66
1:A:367:UFT:H2'	1:A:368:A:H8	1.60	0.66
1:A:213:UFT:H2'	1:A:214:A:H8	1.61	0.66
1:A:91:G:H2'	1:A:92:G:C8	2.30	0.66
1:A:272:UFT:H2'	1:A:273:CFZ:H6	1.78	0.66
1:A:494:A:H3'	1:A:495:A:H5''	1.78	0.66
1:A:271:CFZ:H2'	1:A:272:UFT:H6	1.76	0.66
1:A:97:UFT:H2'	1:A:98:G:H8	1.60	0.66
1:A:451:UFT:H2'	1:A:452:CFZ:H6	1.78	0.66
1:A:502:CFZ:H2'	1:A:503:A:H8	1.61	0.66
1:A:383:UFT:H2'	1:A:384:CFZ:H6	1.78	0.66
1:A:452:CFZ:H2'	1:A:453:CFZ:H6	1.76	0.66
1:A:686:UFT:H2'	1:A:687:UFT:H6	1.78	0.66
1:A:287:CFZ:H2'	1:A:288:UFT:H6	1.77	0.65
1:A:444:UFT:H2'	1:A:445:A:H8	1.61	0.65
1:A:458:CFZ:H2'	1:A:459:A:H8	1.62	0.65
1:A:29:A:N6	1:A:37:A:N6	2.40	0.65
1:A:536:CFZ:H2'	1:A:537:A:H8	1.60	0.65
1:A:83:CFZ:H2'	1:A:84:A:C8	2.31	0.65
1:A:612:UFT:H2'	1:A:613:CFZ:H6	1.78	0.65
1:A:421:UFT:H2'	1:A:422:CFZ:H6	1.79	0.65
1:A:139:G:H2'	1:A:140:G:C8	2.32	0.65
1:A:459:A:N6	1:A:471:UFT:HN3	1.91	0.65
1:A:653:CFZ:H2'	1:A:654:G:H8	1.61	0.64
1:A:332:CFZ:H2'	1:A:333:G:H8	1.62	0.64
1:A:552:A:H2'	1:A:553:G:C8	2.33	0.64
1:A:648:G:O2'	1:A:649:CFZ:O1P	2.16	0.64
1:A:28:CFZ:N3	1:A:38:G:O6	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:CFZ:H2'	1:A:207:A:H8	1.62	0.64
1:A:579:G:H2'	1:A:580:A:C8	2.33	0.64
1:A:46:UFT:H2'	1:A:47:A:C8	2.32	0.63
1:A:156:CFZ:H2'	1:A:157:CFZ:H6	1.81	0.63
1:A:255:G:H2'	1:A:256:CFZ:H6	1.79	0.63
1:A:382:CFZ:H2'	1:A:383:UFT:H6	1.81	0.63
1:A:244:CFZ:H2'	1:A:245:G:H8	1.61	0.63
1:A:123:UFT:H2'	1:A:124:G:H8	1.63	0.63
1:A:361:UFT:H2'	1:A:362:CFZ:H6	1.80	0.63
1:A:354:G:H2'	1:A:355:CFZ:H6	1.81	0.63
1:A:557:CFZ:H2'	1:A:558:UFT:H6	1.80	0.63
1:A:137:CFZ:H2'	1:A:138:UFT:H6	1.78	0.63
1:A:439:CFZ:H2'	1:A:440:G:H8	1.63	0.63
1:A:422:CFZ:H2'	1:A:423:G:H8	1.63	0.62
1:A:425:G:H1	1:A:437:CFZ:HN4	1.47	0.62
1:A:136:A:H2'	1:A:137:CFZ:H6	1.80	0.62
1:A:212:CFZ:H2'	1:A:213:UFT:H6	1.80	0.62
1:A:429:UFT:N3	1:A:430:A:N7	2.46	0.62
1:A:341:A:H2'	1:A:342:CFZ:H6	1.82	0.62
1:A:520:G:H2'	1:A:521:UFT:H6	1.80	0.62
1:A:360:UFT:H2'	1:A:361:UFT:H6	1.80	0.62
1:A:544:G:H2'	1:A:545:A:C8	2.34	0.62
1:A:105:G:H2'	1:A:106:A:H8	1.65	0.62
1:A:215:UFT:H2'	1:A:216:A:C8	2.35	0.62
1:A:323:G:H2'	1:A:324:G:C8	2.34	0.62
1:A:342:CFZ:H2'	1:A:343:CFZ:H6	1.80	0.62
1:A:507:UFT:H2'	1:A:508:G:H8	1.62	0.62
1:A:586:A:N6	1:A:596:G:O6	2.33	0.62
1:A:508:G:H2'	1:A:509:G:H8	1.65	0.61
1:A:512:CFZ:H2'	1:A:513:A:C8	2.34	0.61
1:A:558:UFT:H2'	1:A:559:UFT:H6	1.80	0.61
1:A:559:UFT:H2'	1:A:560:CFZ:H6	1.81	0.61
1:A:215:UFT:H4'	1:A:273:CFZ:H4'	1.82	0.61
1:A:521:UFT:H2'	1:A:522:CFZ:H6	1.83	0.61
1:A:372:G:H2'	1:A:373:A:C8	2.35	0.61
1:A:527:CFZ:H2'	1:A:528:G:C8	2.35	0.61
1:A:363:CFZ:H2'	1:A:364:G:C8	2.36	0.61
1:A:343:CFZ:H2'	1:A:344:CFZ:H6	1.82	0.61
1:A:325:G:H3'	1:A:326:A:H2'	1.83	0.61
1:A:481:G:O2'	1:A:482:G:O5'	2.18	0.61
1:A:161:CFZ:H2'	1:A:162:CFZ:H6	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:UFT:H2'	1:A:341:A:C8	2.35	0.61
1:A:7:CFZ:H2'	1:A:8:A:H8	1.66	0.60
1:A:283:UFT:HN3	1:A:309:A:N6	1.94	0.60
1:A:414:G:H2'	1:A:415:G:C8	2.36	0.60
1:A:668:G:H2'	1:A:669:G:C8	2.36	0.60
1:A:170:UFT:O3'	1:A:172:G:N2	2.34	0.60
1:A:331:A:H2'	1:A:332:CFZ:H6	1.81	0.60
1:A:303:UFT:H2'	1:A:304:G:H8	1.66	0.60
1:A:522:CFZ:H2'	1:A:523:UFT:H6	1.82	0.60
1:A:392:CFZ:H2'	1:A:393:A:H8	1.65	0.60
1:A:111:CFZ:H2'	1:A:112:G:H8	1.65	0.60
1:A:518:CFZ:H2'	1:A:519:G:O4'	2.00	0.60
1:A:99:G:H2'	1:A:100:A:C8	2.36	0.60
1:A:616:UFT:H4'	1:A:617:UFT:H5	1.83	0.60
1:A:625:CFZ:H2'	1:A:626:G:C8	2.37	0.60
1:A:417:UFT:H2'	1:A:418:A:H8	1.67	0.60
1:A:447:G:H2'	1:A:448:G:H8	1.67	0.60
1:A:105:G:H2'	1:A:106:A:C8	2.36	0.59
1:A:647:G:H2'	1:A:648:G:H8	1.66	0.59
1:A:538:CFZ:H2'	1:A:539:G:H8	1.67	0.59
1:A:39:UFT:H2'	1:A:40:G:C8	2.36	0.59
1:A:213:UFT:H2'	1:A:214:A:C8	2.37	0.59
1:A:364:G:H2'	1:A:365:A:C8	2.37	0.59
1:A:339:UFT:H2'	1:A:340:UFT:H6	1.83	0.59
1:A:487:CFZ:H2'	1:A:488:A:H8	1.68	0.59
1:A:455:G:H2'	1:A:456:CFZ:H6	1.83	0.59
1:A:715:A:H3'	1:A:716:UFT:H6	1.84	0.59
1:A:12:CFZ:H2'	1:A:13:A:C8	2.38	0.59
1:A:222:G:O2'	1:A:223:G:OP1	2.19	0.59
1:A:234:CFZ:H2'	1:A:235:A:H8	1.67	0.59
1:A:37:A:O2'	1:A:38:G:H8	1.85	0.59
1:A:190:CFZ:H2'	1:A:191:G:C8	2.37	0.59
1:A:532:UFT:H2'	1:A:533:G:H8	1.68	0.59
1:A:281:A:H2'	1:A:282:G:C8	2.37	0.59
1:A:337:CFZ:H2'	1:A:338:G:C8	2.33	0.59
1:A:544:G:H2'	1:A:545:A:H8	1.68	0.59
1:A:12:CFZ:H2'	1:A:13:A:H8	1.67	0.58
1:A:129:CFZ:O4'	1:A:311:UFT:F2'	2.11	0.58
1:A:364:G:H2'	1:A:365:A:H8	1.68	0.58
1:A:392:CFZ:H2'	1:A:393:A:C8	2.38	0.58
1:A:321:A:O2'	1:A:322:UFT:OP1	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:G:H5''	1:A:326:A:H3'	1.85	0.58
1:A:706:CFZ:H2'	1:A:707:G:H8	1.69	0.58
1:A:1:G:O2'	1:A:2:G:OP1	2.20	0.57
1:A:7:CFZ:H2'	1:A:8:A:C8	2.38	0.57
1:A:206:CFZ:H2'	1:A:207:A:C8	2.40	0.57
1:A:448:G:H2'	1:A:449:G:H8	1.68	0.57
1:A:324:G:H2'	1:A:325:G:C8	2.39	0.57
1:A:43:A:H2'	1:A:44:UFT:H6	1.87	0.57
1:A:609:CFZ:H2'	1:A:610:G:C8	2.39	0.57
1:A:613:CFZ:H2'	1:A:614:G:H8	1.69	0.57
1:A:159:G:O2'	1:A:160:A:OP1	2.22	0.57
1:A:422:CFZ:H2'	1:A:423:G:C8	2.39	0.57
1:A:454:A:H2'	1:A:455:G:H8	1.68	0.57
1:A:689:CFZ:H2'	1:A:690:CFZ:H6	1.87	0.57
1:A:145:G:H2'	1:A:146:CFZ:O4'	2.04	0.57
1:A:217:CFZ:H2'	1:A:218:A:H8	1.69	0.57
1:A:267:UFT:H2'	1:A:268:G:C8	2.39	0.57
1:A:314:CFZ:H2'	1:A:315:A:H8	1.68	0.57
1:A:420:G:H2'	1:A:421:UFT:H6	1.87	0.57
1:A:315:A:N6	1:A:345:UFT:HN3	2.01	0.56
1:A:687:UFT:H2'	1:A:688:G:H8	1.69	0.56
1:A:497:UFT:N3	1:A:498:A:N7	2.54	0.56
1:A:208:CFZ:H2'	1:A:209:CFZ:H6	1.87	0.56
1:A:482:G:H2'	1:A:483:CFZ:H6	1.87	0.56
1:A:18:A:H2'	1:A:19:UFT:H6	1.87	0.56
1:A:83:CFZ:H2'	1:A:84:A:H8	1.70	0.56
1:A:11:CFZ:H2'	1:A:12:CFZ:H6	1.88	0.56
1:A:606:G:C5	1:A:607:UFT:H1'	2.41	0.56
1:A:684:G:O6	1:A:713:CFZ:N3	2.38	0.56
1:A:685:CFZ:H2'	1:A:686:UFT:H6	1.86	0.56
1:A:653:CFZ:H2'	1:A:654:G:C8	2.40	0.56
1:A:417:UFT:H2'	1:A:418:A:C8	2.40	0.56
1:A:502:CFZ:H2'	1:A:503:A:C8	2.40	0.56
1:A:585:UFT:HN3	1:A:586:A:H62	1.52	0.56
1:A:407:CFZ:H2'	1:A:408:G:H8	1.71	0.56
1:A:536:CFZ:H2'	1:A:537:A:C8	2.40	0.56
1:A:2:G:H2'	1:A:3:A:C8	2.42	0.55
1:A:48:UFT:N3	1:A:49:A:C8	2.75	0.55
1:A:437:CFZ:H2'	1:A:438:CFZ:O4'	2.07	0.55
1:A:693:UFT:H2'	1:A:694:CFZ:H6	1.87	0.55
1:A:458:CFZ:H2'	1:A:459:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:G:H2'	1:A:620:CFZ:H6	1.87	0.55
1:A:307:UFT:H2'	1:A:308:CFZ:H6	1.88	0.55
1:A:172:G:H3'	1:A:173:CFZ:H6	1.88	0.55
1:A:359:CFZ:H2'	1:A:360:UFT:H6	1.89	0.55
1:A:565:G:H2'	1:A:566:G:O4'	2.07	0.55
1:A:22:A:H2'	1:A:23:UFT:H6	1.87	0.55
1:A:208:CFZ:H2'	1:A:209:CFZ:C6	2.37	0.55
1:A:448:G:H2'	1:A:449:G:C8	2.41	0.55
1:A:480:UFT:O4	1:A:603:CFZ:N4	2.40	0.55
1:A:714:G:C2	1:A:715:A:C8	2.94	0.55
1:A:94:UFT:H2'	1:A:95:UFT:H6	1.89	0.55
1:A:274:UFT:H2'	1:A:275:CFZ:H6	1.89	0.55
1:A:453:CFZ:H2'	1:A:454:A:H8	1.72	0.55
1:A:175:UFT:H2'	1:A:176:G:C8	2.42	0.55
1:A:218:A:H2'	1:A:219:CFZ:H6	1.89	0.55
1:A:234:CFZ:H2'	1:A:235:A:C8	2.42	0.55
1:A:683:UFT:O5'	1:A:683:UFT:H6	2.07	0.55
1:A:72:CFZ:F2'	1:A:73:CFZ:O4'	2.15	0.54
1:A:20:G:H2'	1:A:21:G:H8	1.71	0.54
1:A:306:CFZ:H2'	1:A:307:UFT:O4'	2.06	0.54
1:A:539:G:H2'	1:A:540:G:H8	1.72	0.54
1:A:50:CFZ:H2'	1:A:51:UFT:H6	1.89	0.54
1:A:323:G:H2'	1:A:324:G:H8	1.70	0.54
1:A:192:UFT:H2'	1:A:193:UFT:H6	1.88	0.54
1:A:21:G:H2'	1:A:22:A:C8	2.43	0.54
1:A:102:G:H2'	1:A:103:CFZ:H6	1.90	0.54
1:A:217:CFZ:H2'	1:A:218:A:C8	2.42	0.54
1:A:267:UFT:H2'	1:A:268:G:H8	1.73	0.54
1:A:367:UFT:H2'	1:A:368:A:C8	2.42	0.54
1:A:432:CFZ:H2'	1:A:433:CFZ:H6	1.89	0.54
1:A:397:UFT:H2'	1:A:398:G:H8	1.73	0.54
1:A:581:G:O2'	1:A:582:UFT:OP1	2.26	0.54
1:A:335:CFZ:H2'	1:A:336:CFZ:C6	2.38	0.54
1:A:439:CFZ:H2'	1:A:440:G:C8	2.42	0.54
1:A:540:G:H2'	1:A:541:CFZ:H6	1.90	0.54
1:A:635:CFZ:H2'	1:A:636:G:H8	1.73	0.54
1:A:687:UFT:H2'	1:A:688:G:C8	2.42	0.54
1:A:226:G:O2'	1:A:227:A:OP1	2.26	0.54
1:A:476:UFT:H2'	1:A:477:G:H8	1.72	0.53
1:A:598:CFZ:H2'	1:A:599:A:H8	1.72	0.53
1:A:635:CFZ:H2'	1:A:636:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:CFZ:H2'	1:A:56:UFT:H6	1.90	0.53
1:A:42:UFT:H2'	1:A:43:A:H8	1.72	0.53
1:A:390:UFT:H2'	1:A:391:CFZ:H6	1.89	0.53
1:A:444:UFT:H2'	1:A:445:A:C8	2.41	0.53
1:A:121:CFZ:H2'	1:A:122:G:C8	2.43	0.53
1:A:110:A:H2'	1:A:111:CFZ:H6	1.91	0.53
1:A:705:UFT:H2'	1:A:706:CFZ:H6	1.90	0.53
1:A:165:CFZ:H2'	1:A:166:A:C8	2.44	0.53
1:A:244:CFZ:H2'	1:A:245:G:C8	2.41	0.53
1:A:214:A:H2'	1:A:215:UFT:H6	1.90	0.53
1:A:258:A:N6	1:A:266:A:H61	2.06	0.53
1:A:470:G:H2'	1:A:471:UFT:H6	1.91	0.53
1:A:508:G:H2'	1:A:509:G:C8	2.43	0.53
1:A:236:UFT:H2'	1:A:237:G:C8	2.45	0.52
1:A:473:CFZ:H2'	1:A:474:G:C8	2.45	0.52
1:A:373:A:H2'	1:A:374:UFT:H6	1.92	0.52
1:A:504:UFT:H2'	1:A:505:G:C8	2.44	0.52
1:A:550:UFT:H2'	1:A:551:G:H8	1.74	0.52
1:A:601:UFT:F2'	1:A:602:CFZ:O4'	2.18	0.52
1:A:32:UFT:HN3	1:A:535:A:H61	1.56	0.52
1:A:44:UFT:H2'	1:A:45:CFZ:H6	1.90	0.52
1:A:406:G:H2'	1:A:407:CFZ:O4'	2.09	0.52
1:A:519:G:H2'	1:A:520:G:C8	2.45	0.52
1:A:706:CFZ:H2'	1:A:707:G:C8	2.44	0.52
1:A:25:G:H2'	1:A:26:CFZ:H6	1.92	0.52
1:A:135:CFZ:H2'	1:A:136:A:H8	1.74	0.52
1:A:188:UFT:HN3	1:A:207:A:N6	2.07	0.52
1:A:204:CFZ:H2'	1:A:205:G:H8	1.75	0.52
1:A:391:CFZ:H2'	1:A:392:CFZ:C6	2.39	0.52
1:A:21:G:H2'	1:A:22:A:H8	1.75	0.51
1:A:567:G:H2'	1:A:568:A:C8	2.46	0.51
1:A:662:UFT:F2'	1:A:663:CFZ:O4'	2.19	0.51
1:A:701:G:N3	1:A:702:G:H1'	2.25	0.51
1:A:618:CFZ:H4'	1:A:619:G:C8	2.46	0.51
1:A:471:UFT:H2'	1:A:472:G:C8	2.46	0.51
1:A:608:G:O6	1:A:628:A:N6	2.43	0.51
1:A:139:G:O6	1:A:149:A:N6	2.43	0.51
1:A:648:G:H2'	1:A:649:CFZ:H6	1.92	0.51
1:A:9:G:H2'	1:A:10:CFZ:H6	1.93	0.51
1:A:165:CFZ:H2'	1:A:166:A:H8	1.75	0.51
1:A:258:A:H61	1:A:266:A:N6	2.05	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:UFT:H2'	1:A:389:G:H8	1.76	0.51
1:A:6:UFT:H2'	1:A:7:CFZ:H6	1.92	0.50
1:A:233:CFZ:H2'	1:A:234:CFZ:H6	1.92	0.50
1:A:336:CFZ:H2'	1:A:337:CFZ:C6	2.41	0.50
1:A:453:CFZ:H2'	1:A:454:A:C8	2.46	0.50
1:A:488:A:H2'	1:A:489:CFZ:H6	1.93	0.50
1:A:520:G:O2'	1:A:521:UFT:OP1	2.25	0.50
1:A:129:CFZ:H5'A	1:A:312:G:H5'	1.93	0.50
1:A:466:CFZ:H2'	1:A:467:CFZ:H6	1.94	0.50
1:A:585:UFT:HN3	1:A:586:A:N6	2.09	0.50
1:A:289:A:C6	1:A:304:G:C6	3.00	0.50
1:A:332:CFZ:H2'	1:A:333:G:C8	2.46	0.50
1:A:447:G:H2'	1:A:448:G:C8	2.46	0.50
1:A:574:CFZ:F2'	1:A:575:UFT:O4'	2.20	0.50
1:A:249:G:H2'	1:A:250:A:H8	1.77	0.50
1:A:440:G:H2'	1:A:441:A:H8	1.76	0.50
1:A:530:A:C8	1:A:531:CFZ:H5	2.46	0.50
1:A:281:A:H2'	1:A:282:G:H8	1.77	0.50
1:A:663:CFZ:N4	1:A:664:G:O6	2.45	0.50
1:A:100:A:H2'	1:A:101:CFZ:H6	1.93	0.50
1:A:546:CFZ:H2'	1:A:547:CFZ:H6	1.93	0.50
1:A:54:A:O2'	1:A:55:CFZ:O1P	2.28	0.50
1:A:93:UFT:H2'	1:A:94:UFT:H6	1.93	0.50
1:A:51:UFT:H2'	1:A:52:G:C8	2.47	0.50
1:A:222:G:H2'	1:A:223:G:C8	2.46	0.50
1:A:366:CFZ:F2'	1:A:367:UFT:O4'	2.20	0.50
1:A:490:CFZ:H2'	1:A:491:G:H8	1.77	0.50
1:A:121:CFZ:N4	1:A:122:G:O6	2.45	0.49
1:A:582:UFT:H2'	1:A:583:G:C8	2.47	0.49
1:A:613:CFZ:H2'	1:A:614:G:C8	2.47	0.49
1:A:703:G:H2'	1:A:704:A:H8	1.77	0.49
1:A:109:CFZ:H2'	1:A:110:A:C8	2.47	0.49
1:A:253:G:H2'	1:A:254:UFT:H6	1.93	0.49
1:A:610:G:H2'	1:A:611:A:C8	2.47	0.49
1:A:456:CFZ:H2'	1:A:457:G:H8	1.77	0.49
1:A:702:G:H3'	1:A:703:G:H5''	1.94	0.49
1:A:723:G:O2'	1:A:724:UFT:OP1	2.29	0.49
1:A:8:A:H2'	1:A:9:G:H8	1.77	0.49
1:A:285:A:H2'	1:A:286:G:H8	1.77	0.49
1:A:291:CFZ:H3'	1:A:292:A:H2'	1.94	0.49
1:A:23:UFT:H2'	1:A:24:A:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:A:H2'	1:A:48:UFT:H6	1.93	0.49
1:A:319:UFT:H2'	1:A:320:A:H8	1.77	0.49
1:A:112:G:H2'	1:A:113:A:C8	2.47	0.49
1:A:111:CFZ:H2'	1:A:112:G:C8	2.45	0.49
1:A:593:G:H2'	1:A:594:CFZ:C6	2.43	0.49
1:A:20:G:H2'	1:A:21:G:C8	2.47	0.49
1:A:246:G:C2	1:A:247:A:C8	3.01	0.49
1:A:581:G:HO2'	1:A:582:UFT:P	2.36	0.49
1:A:459:A:O2'	1:A:460:CFZ:O1P	2.31	0.49
1:A:487:CFZ:H2'	1:A:488:A:C8	2.46	0.49
1:A:619:G:H2'	1:A:620:CFZ:C6	2.43	0.49
1:A:37:A:H62	1:A:531:CFZ:HN4	1.59	0.49
1:A:249:G:H2'	1:A:250:A:C8	2.47	0.49
1:A:637:CFZ:H2'	1:A:638:UFT:H6	1.94	0.49
1:A:723:G:HO2'	1:A:724:UFT:P	2.36	0.49
1:A:133:A:H2'	1:A:134:G:C8	2.47	0.48
1:A:546:CFZ:H2'	1:A:547:CFZ:C6	2.43	0.48
1:A:188:UFT:H2'	1:A:189:G:C8	2.48	0.48
1:A:204:CFZ:H2'	1:A:205:G:C8	2.48	0.48
1:A:78:G:H2'	1:A:79:UFT:H6	1.95	0.48
1:A:324:G:H2'	1:A:325:G:H8	1.78	0.48
1:A:44:UFT:H2'	1:A:45:CFZ:C6	2.44	0.48
1:A:262:G:H2'	1:A:263:UFT:H6	1.95	0.48
1:A:356:UFT:C2	1:A:357:G:C8	2.97	0.48
1:A:372:G:H2'	1:A:373:A:H8	1.75	0.48
1:A:2:G:H2'	1:A:3:A:H8	1.77	0.48
1:A:582:UFT:HN3	1:A:599:A:H61	1.60	0.48
1:A:638:UFT:H2'	1:A:639:A:H8	1.79	0.48
1:A:289:A:N6	1:A:304:G:O6	2.46	0.48
1:A:327:A:C2	1:A:393:A:H1'	2.49	0.48
1:A:520:G:H2'	1:A:521:UFT:C6	2.43	0.48
1:A:28:CFZ:H2'	1:A:29:A:C8	2.48	0.48
1:A:666:CFZ:H2'	1:A:667:UFT:H6	1.95	0.48
1:A:85:A:O2'	1:A:86:A:OP1	2.30	0.47
1:A:495:A:H8	1:A:495:A:OP1	1.97	0.47
1:A:627:UFT:H2'	1:A:628:A:H8	1.79	0.47
1:A:276:CFZ:F2'	1:A:277:UFT:O4'	2.22	0.47
1:A:289:A:H2'	1:A:290:G:H8	1.79	0.47
1:A:657:CFZ:F2'	1:A:658:CFZ:O4'	2.22	0.47
1:A:135:CFZ:H2'	1:A:136:A:C8	2.49	0.47
1:A:174:G:H2'	1:A:175:UFT:H6	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:UFT:H2'	1:A:176:G:H8	1.79	0.47
1:A:407:CFZ:H2'	1:A:408:G:C8	2.49	0.47
1:A:625:CFZ:N4	1:A:626:G:O6	2.47	0.47
1:A:726:G:H3'	1:A:727:UFT:H6	1.96	0.47
1:A:639:A:H2'	1:A:640:G:C8	2.50	0.47
1:A:393:A:H61	1:A:401:A:H61	1.62	0.47
1:A:661:CFZ:F2'	1:A:662:UFT:O4'	2.22	0.47
1:A:215:UFT:H2'	1:A:216:A:H8	1.78	0.47
1:A:286:G:H2'	1:A:287:CFZ:H6	1.96	0.47
1:A:303:UFT:H2'	1:A:304:G:C8	2.49	0.47
1:A:310:CFZ:F2'	1:A:311:UFT:O4'	2.22	0.47
1:A:372:G:O2'	1:A:373:A:OP1	2.31	0.47
1:A:509:G:H2'	1:A:510:UFT:H6	1.96	0.47
1:A:24:A:H2'	1:A:25:G:C8	2.50	0.47
1:A:250:A:H2'	1:A:251:G:C8	2.49	0.47
1:A:539:G:H2'	1:A:540:G:C8	2.50	0.47
1:A:34:CFZ:F2'	1:A:35:A:OP1	2.23	0.47
1:A:250:A:H2'	1:A:251:G:H8	1.80	0.47
1:A:657:CFZ:H6	1:A:657:CFZ:H2'	1.74	0.47
1:A:538:CFZ:H2'	1:A:539:G:C8	2.48	0.47
1:A:566:G:H2'	1:A:567:G:O4'	2.15	0.47
1:A:209:CFZ:H2'	1:A:210:UFT:H6	1.97	0.46
1:A:274:UFT:H2'	1:A:275:CFZ:C6	2.45	0.46
1:A:357:G:C2	1:A:358:G:C8	3.02	0.46
1:A:425:G:O2'	1:A:426:CFZ:H6	2.15	0.46
1:A:517:G:H2'	1:A:518:CFZ:H6	1.97	0.46
1:A:522:CFZ:H2'	1:A:523:UFT:C6	2.45	0.46
1:A:128:CFZ:H6	1:A:128:CFZ:H2'	1.75	0.46
1:A:216:A:H2'	1:A:217:CFZ:H6	1.97	0.46
1:A:319:UFT:H2'	1:A:320:A:C8	2.51	0.46
1:A:339:UFT:H2'	1:A:340:UFT:C6	2.45	0.46
1:A:533:G:O2'	1:A:534:A:OP1	2.28	0.46
1:A:103:CFZ:H2'	1:A:104:CFZ:C6	2.43	0.46
1:A:583:G:H2'	1:A:584:A:H8	1.79	0.46
1:A:352:G:H2'	1:A:353:G:C8	2.51	0.46
1:A:258:A:H4'	1:A:259:A:H5'	1.98	0.46
1:A:113:A:H2'	1:A:114:CFZ:H6	1.97	0.46
1:A:301:G:H2'	1:A:302:CFZ:H6	1.97	0.46
1:A:325:G:OP2	1:A:326:A:O2'	2.32	0.46
1:A:330:CFZ:H4'	1:A:430:A:O2'	2.15	0.46
1:A:365:A:O2'	1:A:366:CFZ:O1P	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:CFZ:H4'	1:A:544:G:O2'	2.16	0.46
1:A:665:CFZ:H2'	1:A:666:CFZ:C6	2.42	0.46
1:A:493:CFZ:F2'	1:A:494:A:O4'	2.24	0.46
1:A:512:CFZ:H2'	1:A:513:A:H8	1.76	0.46
1:A:68:G:C2	1:A:69:A:N7	2.84	0.46
1:A:504:UFT:H2'	1:A:505:G:H8	1.80	0.46
1:A:351:UFT:C2	1:A:352:G:C8	2.99	0.46
1:A:500:CFZ:H2'	1:A:501:UFT:H6	1.97	0.45
1:A:586:A:O2'	1:A:587:G:O4'	2.34	0.45
1:A:694:CFZ:H2'	1:A:695:CFZ:H6	1.98	0.45
1:A:713:CFZ:H2'	1:A:714:G:C8	2.51	0.45
1:A:147:CFZ:F2'	1:A:148:UFT:O4'	2.24	0.45
1:A:219:CFZ:H2'	1:A:220:A:C8	2.51	0.45
1:A:240:UFT:H2'	1:A:241:G:H8	1.80	0.45
1:A:301:G:H2'	1:A:302:CFZ:C6	2.46	0.45
1:A:132:G:H2'	1:A:133:A:C8	2.50	0.45
1:A:173:CFZ:H2'	1:A:174:G:O4'	2.16	0.45
1:A:419:UFT:H2'	1:A:420:G:C8	2.51	0.45
1:A:441:A:H2'	1:A:442:CFZ:H6	1.97	0.45
1:A:560:CFZ:H2'	1:A:561:CFZ:H6	1.99	0.45
1:A:256:CFZ:H2'	1:A:257:A:C8	2.51	0.45
1:A:343:CFZ:H2'	1:A:344:CFZ:C6	2.46	0.45
1:A:666:CFZ:H2'	1:A:667:UFT:C6	2.47	0.45
1:A:33:UFT:H2'	1:A:34:CFZ:H6	1.99	0.45
1:A:109:CFZ:H2'	1:A:110:A:H8	1.81	0.45
1:A:159:G:HO2'	1:A:160:A:P	2.40	0.45
1:A:591:CFZ:H4'	1:A:592:G:C8	2.51	0.45
1:A:707:G:H2'	1:A:708:G:H8	1.81	0.45
1:A:259:A:H4'	1:A:260:A:OP1	2.17	0.45
1:A:399:A:H2'	1:A:400:G:C8	2.52	0.45
1:A:230:UFT:C2	1:A:231:A:C8	3.00	0.45
1:A:541:CFZ:H2'	1:A:542:UFT:C6	2.44	0.44
1:A:154:UFT:F2'	1:A:155:CFZ:O4'	2.25	0.44
1:A:573:UFT:H2'	1:A:574:CFZ:H6	1.99	0.44
1:A:235:A:H2'	1:A:236:UFT:H6	2.00	0.44
1:A:330:CFZ:H2'	1:A:331:A:H8	1.82	0.44
1:A:177:UFT:H2'	1:A:178:CFZ:C6	2.46	0.44
1:A:199:G:H1'	1:A:200:G:C8	2.53	0.44
1:A:450:A:H2'	1:A:451:UFT:H6	1.99	0.44
1:A:468:UFT:H2'	1:A:469:A:H8	1.82	0.44
1:A:275:CFZ:H2'	1:A:276:CFZ:H6	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:A:H2'	1:A:455:G:C8	2.51	0.44
1:A:550:UFT:H2'	1:A:551:G:C8	2.51	0.44
1:A:576:G:O2'	1:A:577:CFZ:H6	2.17	0.44
1:A:713:CFZ:C2	1:A:714:G:C8	3.01	0.44
1:A:191:G:H2'	1:A:192:UFT:H6	1.98	0.44
1:A:54:A:HO2'	1:A:55:CFZ:P	2.40	0.44
1:A:83:CFZ:F2'	1:A:84:A:OP1	2.26	0.44
1:A:171:CFZ:H6	1:A:171:CFZ:H5'	2.00	0.44
1:A:211:G:H2'	1:A:212:CFZ:H6	1.99	0.44
1:A:587:G:H5'	1:A:588:UFT:OP2	2.18	0.44
1:A:257:A:OP2	1:A:258:A:O2'	2.29	0.43
1:A:164:A:H2'	1:A:165:CFZ:H6	1.99	0.43
1:A:210:UFT:H2'	1:A:211:G:O4'	2.18	0.43
1:A:335:CFZ:H2'	1:A:336:CFZ:H6	2.00	0.43
1:A:549:UFT:O5'	1:A:549:UFT:H6	2.18	0.43
1:A:624:UFT:H2'	1:A:625:CFZ:C6	2.48	0.43
1:A:28:CFZ:H6	1:A:28:CFZ:O5'	2.17	0.43
1:A:77:G:C2	1:A:78:G:C8	3.06	0.43
1:A:130:CFZ:H2'	1:A:131:CFZ:O4'	2.18	0.43
1:A:377:UFT:C4	1:A:715:A:N1	2.75	0.43
1:A:586:A:O2'	1:A:587:G:O5'	2.34	0.43
1:A:305:G:H2'	1:A:306:CFZ:H6	2.00	0.43
1:A:430:A:H2'	1:A:431:UFT:H6	2.01	0.43
1:A:117:CFZ:H4'	1:A:118:G:N7	2.34	0.43
1:A:132:G:H2'	1:A:133:A:H8	1.83	0.43
1:A:71:UFT:H2'	1:A:72:CFZ:C6	2.48	0.43
1:A:120:UFT:H2'	1:A:121:CFZ:C6	2.48	0.43
1:A:8:A:H2'	1:A:9:G:C8	2.54	0.43
1:A:42:UFT:H2'	1:A:43:A:C8	2.52	0.43
1:A:230:UFT:H2'	1:A:231:A:H8	1.83	0.43
1:A:45:CFZ:H2'	1:A:46:UFT:C6	2.48	0.43
1:A:171:CFZ:H4'	1:A:173:CFZ:HN4A	1.83	0.43
1:A:338:G:H2'	1:A:339:UFT:H6	2.01	0.43
1:A:499:CFZ:H2'	1:A:500:CFZ:O4'	2.18	0.43
1:A:625:CFZ:H2'	1:A:626:G:H8	1.82	0.43
1:A:650:UFT:C2	1:A:651:A:C8	3.02	0.43
1:A:662:UFT:H2'	1:A:663:CFZ:H6	2.00	0.43
1:A:352:G:H2'	1:A:353:G:H8	1.84	0.43
1:A:519:G:H2'	1:A:520:G:H8	1.84	0.43
1:A:66:UFT:H2'	1:A:67:G:H8	1.84	0.42
1:A:490:CFZ:H2'	1:A:491:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:CFZ:H2'	1:A:220:A:H8	1.84	0.42
1:A:485:UFT:H2'	1:A:486:G:O4'	2.19	0.42
1:A:521:UFT:F2'	1:A:522:CFZ:O4'	2.27	0.42
1:A:363:CFZ:H2'	1:A:364:G:H8	1.79	0.42
1:A:636:G:H2'	1:A:637:CFZ:H6	2.00	0.42
1:A:69:A:C2	1:A:70:G:C8	3.07	0.42
1:A:136:A:N6	1:A:152:G:C6	2.88	0.42
1:A:275:CFZ:H2'	1:A:276:CFZ:C6	2.50	0.42
1:A:623:A:H2'	1:A:624:UFT:H6	2.02	0.42
1:A:674:CFZ:H2'	1:A:675:CFZ:C6	2.49	0.42
1:A:680:G:H2'	1:A:681:A:C8	2.55	0.42
1:A:713:CFZ:H2'	1:A:714:G:H8	1.83	0.42
1:A:330:CFZ:H2'	1:A:331:A:C8	2.55	0.42
1:A:365:A:H2'	1:A:366:CFZ:C6	2.50	0.42
1:A:440:G:H2'	1:A:441:A:C8	2.53	0.42
1:A:247:A:H2'	1:A:248:G:C8	2.53	0.42
1:A:382:CFZ:HN4	1:A:412:G:H1	1.66	0.42
1:A:36:G:H5'	1:A:37:A:OP2	2.20	0.42
1:A:133:A:H2'	1:A:134:G:H8	1.85	0.42
1:A:80:CFZ:H2'	1:A:81:CFZ:H6	2.02	0.42
1:A:382:CFZ:H2'	1:A:383:UFT:C6	2.48	0.42
1:A:153:CFZ:F2'	1:A:154:UFT:O4'	2.28	0.42
1:A:192:UFT:H2'	1:A:193:UFT:C6	2.50	0.42
1:A:346:CFZ:F2'	1:A:347:G:OP1	2.27	0.42
1:A:184:CFZ:H6	1:A:184:CFZ:O5'	2.20	0.42
1:A:1:G:HO2'	1:A:2:G:P	2.41	0.41
1:A:419:UFT:H2'	1:A:420:G:H8	1.84	0.41
1:A:491:G:H2'	1:A:492:G:O4'	2.20	0.41
1:A:97:UFT:F2'	1:A:98:G:OP1	2.28	0.41
1:A:255:G:H2'	1:A:256:CFZ:C6	2.46	0.41
1:A:350:UFT:H2'	1:A:351:UFT:C6	2.48	0.41
1:A:380:G:H2'	1:A:381:G:O4'	2.20	0.41
1:A:567:G:H2'	1:A:568:A:H8	1.84	0.41
1:A:66:UFT:H2'	1:A:67:G:C8	2.55	0.41
1:A:283:UFT:F2'	1:A:341:A:H5'	2.10	0.41
1:A:427:A:H61	1:A:435:A:H61	1.67	0.41
1:A:596:G:C6	1:A:597:UFT:C4	3.03	0.41
1:A:722:G:N3	1:A:723:G:C8	2.89	0.41
1:A:329:UFT:H2'	1:A:330:CFZ:H6	2.03	0.41
1:A:704:A:H3'	1:A:705:UFT:H6	2.03	0.41
1:A:706:CFZ:C2	1:A:707:G:C8	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:CFZ:H2'	1:A:11:CFZ:H6	2.02	0.41
1:A:222:G:O3'	1:A:224:A:O2'	2.34	0.41
1:A:416:CFZ:H2'	1:A:417:UFT:C6	2.48	0.41
1:A:622:G:H2'	1:A:623:A:C8	2.56	0.41
1:A:634:A:H2'	1:A:635:CFZ:H6	2.02	0.41
1:A:647:G:H2'	1:A:648:G:C8	2.51	0.41
1:A:35:A:N6	1:A:533:G:O6	2.53	0.41
1:A:94:UFT:H2'	1:A:95:UFT:C6	2.49	0.41
1:A:214:A:H61	1:A:242:UFT:HN3	1.67	0.41
1:A:226:G:HO2'	1:A:227:A:P	2.44	0.41
1:A:249:G:O2'	1:A:306:CFZ:H4'	2.20	0.41
1:A:508:G:C2	1:A:509:G:C5	3.09	0.41
1:A:593:G:H2'	1:A:594:CFZ:H6	2.03	0.41
1:A:594:CFZ:H6	1:A:594:CFZ:O5'	2.20	0.41
1:A:67:G:H2'	1:A:68:G:H8	1.85	0.41
1:A:353:G:H2'	1:A:354:G:H8	1.85	0.41
1:A:459:A:HO2'	1:A:460:CFZ:P	2.41	0.41
1:A:608:G:H2'	1:A:609:CFZ:H6	2.02	0.41
1:A:650:UFT:H2'	1:A:651:A:H8	1.86	0.41
1:A:24:A:H2'	1:A:25:G:H8	1.85	0.41
1:A:575:UFT:H6	1:A:575:UFT:H2'	1.86	0.41
1:A:688:G:H2'	1:A:689:CFZ:H6	2.03	0.41
1:A:106:A:H2'	1:A:107:UFT:O4'	2.21	0.40
1:A:252:A:H2'	1:A:253:G:H8	1.86	0.40
1:A:289:A:H2'	1:A:290:G:C8	2.57	0.40
1:A:340:UFT:C2	1:A:341:A:C8	3.04	0.40
1:A:342:CFZ:H2'	1:A:343:CFZ:C6	2.47	0.40
1:A:372:G:N1	1:A:721:A:N6	2.69	0.40
1:A:452:CFZ:H2'	1:A:453:CFZ:C6	2.48	0.40
1:A:588:UFT:H5'	1:A:589:UFT:OP2	2.22	0.40
1:A:724:UFT:C2	1:A:725:A:C8	3.05	0.40
1:A:157:CFZ:H2'	1:A:158:G:H8	1.86	0.40
1:A:302:CFZ:H6	1:A:302:CFZ:O5'	2.21	0.40
1:A:372:G:O2'	1:A:373:A:P	2.79	0.40
1:A:533:G:C2	1:A:534:A:N7	2.89	0.40
1:A:681:A:H2'	1:A:682:G:C8	2.55	0.40
1:A:247:A:H61	1:A:277:UFT:HN3	1.69	0.40
1:A:129:CFZ:H2'	1:A:130:CFZ:H6	2.03	0.40
1:A:474:G:H2'	1:A:475:UFT:O4'	2.22	0.40
1:A:534:A:H2'	1:A:535:A:O4'	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	196/728 (26%)	76 (38%)	15 (7%)

All (76) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	30	A
1	A	31	G
1	A	37	A
1	A	38	G
1	A	53	G
1	A	60	G
1	A	68	G
1	A	69	A
1	A	70	G
1	A	85	A
1	A	86	A
1	A	99	G
1	A	119	G
1	A	160	A
1	A	186	G
1	A	200	G
1	A	202	A
1	A	223	G
1	A	225	A
1	A	226	G
1	A	227	A
1	A	248	G
1	A	251	G
1	A	258	A

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Mol	Chain	Res	Type
1	A	259	A
1	A	260	A
1	A	266	A
1	A	296	G
1	A	297	A
1	A	301	G
1	A	313	G
1	A	316	G
1	A	317	G
1	A	321	A
1	A	325	G
1	A	327	A
1	A	348	G
1	A	373	A
1	A	399	A
1	A	403	G
1	A	404	A
1	A	411	A
1	A	413	G
1	A	414	G
1	A	425	G
1	A	428	A
1	A	436	G
1	A	447	G
1	A	462	A
1	A	482	G
1	A	492	G
1	A	495	A
1	A	517	G
1	A	530	A
1	A	534	A
1	A	535	A
1	A	540	G
1	A	566	G
1	A	567	G
1	A	568	A
1	A	569	A
1	A	572	G
1	A	580	A
1	A	581	G
1	A	584	A
1	A	615	G

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Mol	Chain	Res	Type
1	A	647	G
1	A	660	A
1	A	702	G
1	A	703	G
1	A	708	G
1	A	711	A
1	A	712	G
1	A	715	A
1	A	723	G

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1	G
1	A	30	A
1	A	67	G
1	A	85	A
1	A	159	G
1	A	222	G
1	A	226	G
1	A	250	A
1	A	372	G
1	A	427	A
1	A	533	G
1	A	539	G
1	A	567	G
1	A	583	G
1	A	707	G

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

361 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	CFZ	A	161	1	18,21,22	2.51	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	11	1	18,21,22	2.52	7 (38%)	25,30,33	1.58	2 (8%)
1	CFZ	A	378	1	18,21,22	2.45	7 (38%)	25,30,33	1.56	3 (12%)
1	UFT	A	485	1	18,21,22	2.67	10 (55%)	25,30,33	2.01	6 (24%)
1	UFT	A	409	1	18,21,22	2.67	10 (55%)	25,30,33	2.20	7 (28%)
1	CFZ	A	717	1	18,21,22	2.45	6 (33%)	25,30,33	1.61	2 (8%)
1	CFZ	A	426	1	18,21,22	2.45	7 (38%)	25,30,33	1.34	3 (12%)
1	UFT	A	542	1	18,21,22	2.62	10 (55%)	25,30,33	2.14	8 (32%)
1	CFZ	A	632	1	18,21,22	2.54	6 (33%)	25,30,33	1.36	3 (12%)
1	CFZ	A	661	1	18,21,22	2.50	7 (38%)	25,30,33	1.35	3 (12%)
1	UFT	A	595	1	18,21,22	2.60	10 (55%)	25,30,33	2.16	6 (24%)
1	UFT	A	627	1	18,21,22	2.65	10 (55%)	25,30,33	1.88	5 (20%)
1	CFZ	A	405	1	18,21,22	2.50	7 (38%)	25,30,33	1.23	3 (12%)
1	CFZ	A	346	1	18,21,22	2.44	7 (38%)	25,30,33	1.52	3 (12%)
1	UFT	A	670	1	18,21,22	2.61	10 (55%)	25,30,33	2.05	8 (32%)
1	CFZ	A	128	1	18,21,22	2.45	7 (38%)	25,30,33	1.44	3 (12%)
1	UFT	A	236	1	18,21,22	2.66	10 (55%)	25,30,33	2.17	7 (28%)
1	CFZ	A	658	1	18,21,22	2.47	7 (38%)	25,30,33	1.56	3 (12%)
1	CFZ	A	206	1	18,21,22	2.47	7 (38%)	25,30,33	1.37	2 (8%)
1	CFZ	A	275	1	18,21,22	2.54	7 (38%)	25,30,33	1.38	2 (8%)
1	UFT	A	61	1	18,21,22	2.63	10 (55%)	25,30,33	2.09	8 (32%)
1	UFT	A	51	1	18,21,22	2.69	10 (55%)	25,30,33	2.33	7 (28%)
1	CFZ	A	577	1	18,21,22	2.50	6 (33%)	25,30,33	1.34	3 (12%)
1	UFT	A	95	1	18,21,22	2.59	10 (55%)	25,30,33	2.13	7 (28%)
1	UFT	A	283	1	18,21,22	2.67	10 (55%)	25,30,33	2.26	7 (28%)
1	CFZ	A	518	1	18,21,22	2.55	6 (33%)	25,30,33	1.24	2 (8%)
1	UFT	A	471	1	18,21,22	2.72	10 (55%)	25,30,33	2.38	7 (28%)
1	UFT	A	329	1	18,21,22	2.64	9 (50%)	25,30,33	2.12	7 (28%)
1	CFZ	A	45	1	18,21,22	2.54	7 (38%)	25,30,33	1.29	2 (8%)
1	UFT	A	687	1	18,21,22	2.68	10 (55%)	25,30,33	2.09	7 (28%)
1	CFZ	A	72	1	18,21,22	2.51	7 (38%)	25,30,33	1.28	2 (8%)
1	UFT	A	196	1	18,21,22	2.57	10 (55%)	25,30,33	2.07	7 (28%)
1	CFZ	A	675	1	18,21,22	2.49	7 (38%)	25,30,33	1.47	2 (8%)
1	UFT	A	175	1	18,21,22	2.61	10 (55%)	25,30,33	1.98	7 (28%)
1	CFZ	A	63	1	18,21,22	2.48	7 (38%)	25,30,33	1.54	3 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	UFT	A	475	1	18,21,22	2.62	8 (44%)	25,30,33	2.12	7 (28%)
1	UFT	A	667	1	18,21,22	2.57	9 (50%)	25,30,33	2.06	7 (28%)
1	CFZ	A	50	1	18,21,22	2.51	6 (33%)	25,30,33	1.63	3 (12%)
1	UFT	A	585	1	18,21,22	2.62	10 (55%)	25,30,33	2.17	7 (28%)
1	CFZ	A	165	1	18,21,22	2.52	6 (33%)	25,30,33	1.46	2 (8%)
1	UFT	A	56	1	18,21,22	2.68	10 (55%)	25,30,33	2.27	8 (32%)
1	CFZ	A	433	1	18,21,22	2.50	7 (38%)	25,30,33	1.37	3 (12%)
1	UFT	A	575	1	18,21,22	2.68	10 (55%)	25,30,33	2.17	8 (32%)
1	UFT	A	444	1	18,21,22	2.60	9 (50%)	25,30,33	1.91	7 (28%)
1	UFT	A	650	1	18,21,22	2.65	10 (55%)	25,30,33	2.36	8 (32%)
1	UFT	A	115	1	18,21,22	2.63	10 (55%)	25,30,33	2.06	7 (28%)
1	CFZ	A	195	1	18,21,22	2.48	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	75	1	18,21,22	2.52	7 (38%)	25,30,33	1.47	3 (12%)
1	CFZ	A	602	1	18,21,22	2.50	7 (38%)	25,30,33	1.47	5 (20%)
1	UFT	A	683	1	18,21,22	2.59	10 (55%)	25,30,33	2.24	7 (28%)
1	CFZ	A	137	1	18,21,22	2.55	7 (38%)	25,30,33	1.36	2 (8%)
1	CFZ	A	500	1	18,21,22	2.44	7 (38%)	25,30,33	1.47	3 (12%)
1	CFZ	A	416	1	18,21,22	2.54	6 (33%)	25,30,33	1.42	3 (12%)
1	UFT	A	607	1	18,21,22	2.67	10 (55%)	25,30,33	2.37	6 (24%)
1	CFZ	A	101	1	18,21,22	2.50	6 (33%)	25,30,33	1.41	2 (8%)
1	CFZ	A	184	1	18,21,22	2.50	6 (33%)	25,30,33	1.39	3 (12%)
1	UFT	A	298	1	18,21,22	2.64	9 (50%)	25,30,33	1.89	5 (20%)
1	CFZ	A	460	1	18,21,22	2.46	7 (38%)	25,30,33	1.39	2 (8%)
1	CFZ	A	578	1	18,21,22	2.51	7 (38%)	25,30,33	1.63	3 (12%)
1	CFZ	A	233	1	18,21,22	2.53	7 (38%)	25,30,33	1.37	3 (12%)
1	CFZ	A	355	1	18,21,22	2.53	7 (38%)	25,30,33	1.27	2 (8%)
1	CFZ	A	442	1	18,21,22	2.48	7 (38%)	25,30,33	1.49	3 (12%)
1	UFT	A	193	1	18,21,22	2.62	10 (55%)	25,30,33	2.07	7 (28%)
1	CFZ	A	308	1	18,21,22	2.55	6 (33%)	25,30,33	1.23	2 (8%)
1	CFZ	A	609	1	18,21,22	2.51	7 (38%)	25,30,33	1.43	2 (8%)
1	UFT	A	62	1	18,21,22	2.59	10 (55%)	25,30,33	2.16	8 (32%)
1	UFT	A	311	1	18,21,22	2.69	10 (55%)	25,30,33	2.19	9 (36%)
1	CFZ	A	649	1	18,21,22	2.54	6 (33%)	25,30,33	1.32	2 (8%)
1	UFT	A	464	1	18,21,22	2.63	10 (55%)	25,30,33	2.18	8 (32%)
1	CFZ	A	337	1	18,21,22	2.56	7 (38%)	25,30,33	1.14	2 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CFZ	A	618	1	18,21,22	2.46	7 (38%)	25,30,33	1.49	2 (8%)
1	UFT	A	221	1	18,21,22	2.69	9 (50%)	25,30,33	1.92	6 (24%)
1	UFT	A	727	1	18,21,22	2.66	9 (50%)	25,30,33	2.03	8 (32%)
1	CFZ	A	57	1	18,21,22	2.56	7 (38%)	25,30,33	1.43	3 (12%)
1	CFZ	A	621	1	18,21,22	2.47	7 (38%)	25,30,33	1.49	3 (12%)
1	CFZ	A	392	1	18,21,22	2.47	7 (38%)	25,30,33	1.36	3 (12%)
1	UFT	A	274	1	18,21,22	2.65	10 (55%)	25,30,33	2.04	7 (28%)
1	UFT	A	679	1	18,21,22	2.63	10 (55%)	25,30,33	2.21	6 (24%)
1	CFZ	A	637	1	18,21,22	2.49	7 (38%)	25,30,33	1.28	2 (8%)
1	UFT	A	93	1	18,21,22	2.65	10 (55%)	25,30,33	2.19	7 (28%)
1	UFT	A	194	1	18,21,22	2.71	10 (55%)	25,30,33	2.33	7 (28%)
1	UFT	A	154	1	18,21,22	2.62	9 (50%)	25,30,33	2.11	10 (40%)
1	UFT	A	215	1	18,21,22	2.66	9 (50%)	25,30,33	2.01	6 (24%)
1	CFZ	A	144	1	18,21,22	2.49	7 (38%)	25,30,33	1.13	1 (4%)
1	CFZ	A	382	1	18,21,22	2.54	6 (33%)	25,30,33	1.35	2 (8%)
1	CFZ	A	162	1	18,21,22	2.53	7 (38%)	25,30,33	1.28	2 (8%)
1	CFZ	A	90	1	18,21,22	2.45	7 (38%)	25,30,33	1.34	2 (8%)
1	CFZ	A	129	1	18,21,22	2.53	7 (38%)	25,30,33	1.39	2 (8%)
1	CFZ	A	111	1	18,21,22	2.52	7 (38%)	25,30,33	1.35	3 (12%)
1	UFT	A	556	1	18,21,22	2.64	10 (55%)	25,30,33	2.05	6 (24%)
1	CFZ	A	506	1	18,21,22	2.51	7 (38%)	25,30,33	1.30	2 (8%)
1	UFT	A	138	1	18,21,22	2.61	10 (55%)	25,30,33	2.12	8 (32%)
1	UFT	A	127	1	18,21,22	2.61	10 (55%)	25,30,33	2.18	8 (32%)
1	CFZ	A	332	1	18,21,22	2.55	6 (33%)	25,30,33	1.28	2 (8%)
1	CFZ	A	391	1	18,21,22	2.49	6 (33%)	25,30,33	1.53	2 (8%)
1	CFZ	A	15	1	18,21,22	2.48	7 (38%)	25,30,33	1.54	3 (12%)
1	UFT	A	724	1	18,21,22	2.57	9 (50%)	25,30,33	1.98	6 (24%)
1	CFZ	A	656	1	18,21,22	2.47	7 (38%)	25,30,33	1.50	3 (12%)
1	CFZ	A	153	1	18,21,22	2.52	7 (38%)	25,30,33	1.42	2 (8%)
1	UFT	A	48	1	18,21,22	2.69	9 (50%)	25,30,33	1.93	7 (28%)
1	CFZ	A	483	1	18,21,22	2.51	7 (38%)	25,30,33	1.25	2 (8%)
1	CFZ	A	438	1	18,21,22	2.48	7 (38%)	25,30,33	1.32	2 (8%)
1	CFZ	A	515	1	18,21,22	2.50	6 (33%)	25,30,33	1.80	6 (24%)
1	UFT	A	388	1	18,21,22	2.64	10 (55%)	25,30,33	2.08	6 (24%)
1	UFT	A	698	1	18,21,22	2.61	10 (55%)	25,30,33	2.07	7 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	UFT	A	116	1	18,21,22	2.63	10 (55%)	25,30,33	1.94	5 (20%)
1	UFT	A	169	1	18,21,22	2.61	9 (50%)	25,30,33	2.19	7 (28%)
1	UFT	A	360	1	18,21,22	2.67	9 (50%)	25,30,33	2.08	7 (28%)
1	UFT	A	123	1	18,21,22	2.63	10 (55%)	25,30,33	2.15	7 (28%)
1	CFZ	A	526	1	18,21,22	2.51	7 (38%)	25,30,33	1.61	4 (16%)
1	CFZ	A	208	1	18,21,22	2.54	7 (38%)	25,30,33	1.41	3 (12%)
1	CFZ	A	641	1	18,21,22	2.49	7 (38%)	25,30,33	1.24	2 (8%)
1	UFT	A	451	1	18,21,22	2.65	9 (50%)	25,30,33	1.95	6 (24%)
1	CFZ	A	439	1	18,21,22	2.55	7 (38%)	25,30,33	1.26	3 (12%)
1	CFZ	A	690	1	18,21,22	2.48	7 (38%)	25,30,33	1.43	2 (8%)
1	CFZ	A	121	1	18,21,22	2.50	7 (38%)	25,30,33	1.24	3 (12%)
1	UFT	A	345	1	18,21,22	2.60	10 (55%)	25,30,33	2.06	7 (28%)
1	CFZ	A	108	1	18,21,22	2.55	7 (38%)	25,30,33	1.35	2 (8%)
1	CFZ	A	456	1	18,21,22	2.52	7 (38%)	25,30,33	1.32	3 (12%)
1	UFT	A	417	1	18,21,22	2.61	9 (50%)	25,30,33	1.93	7 (28%)
1	CFZ	A	330	1	18,21,22	2.52	7 (38%)	25,30,33	1.44	4 (16%)
1	UFT	A	361	1	18,21,22	2.58	9 (50%)	25,30,33	2.15	7 (28%)
1	UFT	A	350	1	18,21,22	2.66	10 (55%)	25,30,33	2.01	6 (24%)
1	UFT	A	319	1	18,21,22	2.62	9 (50%)	25,30,33	2.05	6 (24%)
1	CFZ	A	502	1	18,21,22	2.46	7 (38%)	25,30,33	1.48	4 (16%)
1	UFT	A	573	1	18,21,22	2.69	9 (50%)	25,30,33	2.13	7 (28%)
1	CFZ	A	625	1	18,21,22	2.51	7 (38%)	25,30,33	1.19	2 (8%)
1	UFT	A	240	1	18,21,22	2.61	10 (55%)	25,30,33	2.08	8 (32%)
1	CFZ	A	466	1	18,21,22	2.55	7 (38%)	25,30,33	1.27	3 (12%)
1	CFZ	A	603	1	18,21,22	2.47	7 (38%)	25,30,33	1.56	3 (12%)
1	UFT	A	555	1	18,21,22	2.66	10 (55%)	25,30,33	1.93	6 (24%)
1	CFZ	A	190	1	18,21,22	2.54	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	384	1	18,21,22	2.55	7 (38%)	25,30,33	1.33	2 (8%)
1	CFZ	A	452	1	18,21,22	2.54	7 (38%)	25,30,33	1.26	2 (8%)
1	CFZ	A	657	1	18,21,22	2.49	7 (38%)	25,30,33	1.47	4 (16%)
1	CFZ	A	473	1	18,21,22	2.46	7 (38%)	25,30,33	1.21	2 (8%)
1	UFT	A	612	1	18,21,22	2.69	10 (55%)	25,30,33	2.05	5 (20%)
1	CFZ	A	674	1	18,21,22	2.49	7 (38%)	25,30,33	1.49	2 (8%)
1	CFZ	A	103	1	18,21,22	2.51	6 (33%)	25,30,33	1.25	2 (8%)
1	CFZ	A	557	1	18,21,22	2.54	6 (33%)	25,30,33	1.54	3 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	UFT	A	307	1	18,21,22	2.64	9 (50%)	25,30,33	1.87	6 (24%)
1	CFZ	A	709	1	18,21,22	2.51	6 (33%)	25,30,33	1.55	5 (20%)
1	CFZ	A	273	1	18,21,22	2.50	6 (33%)	25,30,33	1.45	2 (8%)
1	UFT	A	532	1	18,21,22	2.55	9 (50%)	25,30,33	1.90	8 (32%)
1	UFT	A	497	1	18,21,22	2.71	9 (50%)	25,30,33	2.16	8 (32%)
1	CFZ	A	538	1	18,21,22	2.56	7 (38%)	25,30,33	1.26	3 (12%)
1	UFT	A	601	1	18,21,22	2.64	10 (55%)	25,30,33	2.41	9 (36%)
1	CFZ	A	28	1	18,21,22	2.47	7 (38%)	25,30,33	1.52	6 (24%)
1	CFZ	A	629	1	18,21,22	2.43	7 (38%)	25,30,33	1.74	5 (20%)
1	UFT	A	167	1	18,21,22	2.62	10 (55%)	25,30,33	2.07	8 (32%)
1	CFZ	A	695	1	18,21,22	2.52	6 (33%)	25,30,33	1.36	3 (12%)
1	UFT	A	177	1	18,21,22	2.64	10 (55%)	25,30,33	2.12	7 (28%)
1	UFT	A	23	1	18,21,22	2.75	10 (55%)	25,30,33	2.10	6 (24%)
1	CFZ	A	209	1	18,21,22	2.54	6 (33%)	25,30,33	1.30	3 (12%)
1	CFZ	A	156	1	18,21,22	2.54	7 (38%)	25,30,33	1.27	2 (8%)
1	UFT	A	642	1	18,21,22	2.62	9 (50%)	25,30,33	1.89	6 (24%)
1	UFT	A	170	1	18,21,22	2.65	10 (55%)	25,30,33	2.00	7 (28%)
1	UFT	A	671	1	18,21,22	2.61	10 (55%)	25,30,33	2.15	7 (28%)
1	CFZ	A	104	1	18,21,22	2.54	7 (38%)	25,30,33	1.20	2 (8%)
1	UFT	A	397	1	18,21,22	2.63	10 (55%)	25,30,33	2.09	8 (32%)
1	UFT	A	510	1	18,21,22	2.59	9 (50%)	25,30,33	2.13	7 (28%)
1	UFT	A	89	1	18,21,22	2.59	10 (55%)	25,30,33	2.17	8 (32%)
1	CFZ	A	594	1	18,21,22	2.51	7 (38%)	25,30,33	1.43	2 (8%)
1	UFT	A	419	1	18,21,22	2.68	9 (50%)	25,30,33	1.95	7 (28%)
1	CFZ	A	335	1	18,21,22	2.53	6 (33%)	25,30,33	1.61	4 (16%)
1	UFT	A	197	1	18,21,22	2.63	10 (55%)	25,30,33	2.06	8 (32%)
1	CFZ	A	379	1	18,21,22	2.56	8 (44%)	25,30,33	1.33	4 (16%)
1	CFZ	A	685	1	18,21,22	2.50	7 (38%)	25,30,33	1.58	2 (8%)
1	CFZ	A	12	1	18,21,22	2.56	7 (38%)	25,30,33	1.38	2 (8%)
1	CFZ	A	306	1	18,21,22	2.54	6 (33%)	25,30,33	1.20	1 (4%)
1	UFT	A	39	1	18,21,22	2.65	9 (50%)	25,30,33	1.76	6 (24%)
1	CFZ	A	363	1	18,21,22	2.55	7 (38%)	25,30,33	1.29	2 (8%)
1	CFZ	A	467	1	18,21,22	2.53	7 (38%)	25,30,33	1.31	2 (8%)
1	CFZ	A	366	1	18,21,22	2.54	7 (38%)	25,30,33	1.36	4 (16%)
1	CFZ	A	604	1	18,21,22	2.51	7 (38%)	25,30,33	1.15	1 (4%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CFZ	A	696	1	18,21,22	2.53	6 (33%)	25,30,33	1.23	2 (8%)
1	UFT	A	263	1	18,21,22	2.64	10 (55%)	25,30,33	2.18	8 (32%)
1	CFZ	A	310	1	18,21,22	2.58	7 (38%)	25,30,33	1.41	3 (12%)
1	UFT	A	476	1	18,21,22	2.63	10 (55%)	25,30,33	2.05	6 (24%)
1	UFT	A	590	1	18,21,22	2.60	9 (50%)	25,30,33	2.12	8 (32%)
1	UFT	A	272	1	18,21,22	2.62	9 (50%)	25,30,33	1.98	6 (24%)
1	CFZ	A	157	1	18,21,22	2.47	7 (38%)	25,30,33	1.39	3 (12%)
1	CFZ	A	395	1	18,21,22	2.50	7 (38%)	25,30,33	1.35	3 (12%)
1	CFZ	A	7	1	18,21,22	2.56	7 (38%)	25,30,33	1.25	2 (8%)
1	UFT	A	597	1	18,21,22	2.63	10 (55%)	25,30,33	2.11	7 (28%)
1	UFT	A	521	1	18,21,22	2.64	10 (55%)	25,30,33	2.12	9 (36%)
1	UFT	A	351	1	18,21,22	2.56	10 (55%)	25,30,33	2.00	8 (32%)
1	CFZ	A	487	1	18,21,22	2.53	7 (38%)	25,30,33	1.39	4 (16%)
1	CFZ	A	598	1	18,21,22	2.53	7 (38%)	25,30,33	1.51	3 (12%)
1	CFZ	A	631	1	18,21,22	2.57	7 (38%)	25,30,33	1.27	2 (8%)
1	CFZ	A	434	1	18,21,22	2.57	6 (33%)	25,30,33	1.26	3 (12%)
1	CFZ	A	212	1	18,21,22	2.54	6 (33%)	25,30,33	1.42	3 (12%)
1	CFZ	A	155	1	18,21,22	2.46	7 (38%)	25,30,33	1.47	4 (16%)
1	UFT	A	480	1	18,21,22	2.59	9 (50%)	25,30,33	2.08	7 (28%)
1	UFT	A	242	1	18,21,22	2.61	10 (55%)	25,30,33	2.15	7 (28%)
1	CFZ	A	531	1	18,21,22	2.47	6 (33%)	25,30,33	1.57	2 (8%)
1	UFT	A	662	1	18,21,22	2.65	10 (55%)	25,30,33	2.10	9 (36%)
1	CFZ	A	302	1	18,21,22	2.54	7 (38%)	25,30,33	1.36	2 (8%)
1	CFZ	A	369	1	18,21,22	2.52	7 (38%)	25,30,33	1.31	2 (8%)
1	CFZ	A	26	1	18,21,22	2.48	7 (38%)	25,30,33	1.33	3 (12%)
1	UFT	A	377	1	18,21,22	2.75	9 (50%)	25,30,33	2.69	10 (40%)
1	CFZ	A	234	1	18,21,22	2.56	7 (38%)	25,30,33	1.38	2 (8%)
1	CFZ	A	343	1	18,21,22	2.53	7 (38%)	25,30,33	1.25	2 (8%)
1	UFT	A	356	1	18,21,22	2.61	10 (55%)	25,30,33	2.14	6 (24%)
1	CFZ	A	564	1	18,21,22	2.47	7 (38%)	25,30,33	1.23	2 (8%)
1	CFZ	A	76	1	18,21,22	2.53	7 (38%)	25,30,33	1.28	1 (4%)
1	CFZ	A	574	1	18,21,22	2.50	7 (38%)	25,30,33	1.33	3 (12%)
1	CFZ	A	699	1	18,21,22	2.49	7 (38%)	25,30,33	1.29	2 (8%)
1	UFT	A	563	1	18,21,22	2.62	10 (55%)	25,30,33	2.08	8 (32%)
1	CFZ	A	130	1	18,21,22	2.52	7 (38%)	25,30,33	1.27	3 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CFZ	A	432	1	18,21,22	2.51	7 (38%)	25,30,33	1.45	3 (12%)
1	UFT	A	421	1	18,21,22	2.64	10 (55%)	25,30,33	2.01	7 (28%)
1	CFZ	A	666	1	18,21,22	2.53	6 (33%)	25,30,33	1.45	2 (8%)
1	CFZ	A	117	1	18,21,22	2.47	7 (38%)	25,30,33	1.46	3 (12%)
1	UFT	A	367	1	18,21,22	2.71	10 (55%)	25,30,33	2.27	6 (24%)
1	CFZ	A	437	1	18,21,22	2.57	7 (38%)	25,30,33	1.34	2 (8%)
1	UFT	A	66	1	18,21,22	2.69	10 (55%)	25,30,33	2.25	8 (32%)
1	CFZ	A	109	1	18,21,22	2.54	6 (33%)	25,30,33	1.53	4 (16%)
1	UFT	A	210	1	18,21,22	2.70	10 (55%)	25,30,33	2.17	8 (32%)
1	UFT	A	288	1	18,21,22	2.65	10 (55%)	25,30,33	2.12	6 (24%)
1	CFZ	A	489	1	18,21,22	2.51	7 (38%)	25,30,33	1.25	3 (12%)
1	UFT	A	142	1	18,21,22	2.59	10 (55%)	25,30,33	2.07	7 (28%)
1	UFT	A	719	1	18,21,22	2.60	9 (50%)	25,30,33	2.01	7 (28%)
1	CFZ	A	512	1	18,21,22	2.53	7 (38%)	25,30,33	1.35	2 (8%)
1	CFZ	A	453	1	18,21,22	2.52	7 (38%)	25,30,33	1.31	2 (8%)
1	CFZ	A	386	1	18,21,22	2.50	7 (38%)	25,30,33	1.40	3 (12%)
1	CFZ	A	600	1	18,21,22	2.56	6 (33%)	25,30,33	1.36	2 (8%)
1	CFZ	A	728	1	18,21,22	2.46	7 (38%)	25,30,33	1.36	3 (12%)
1	CFZ	A	605	1	18,21,22	2.51	7 (38%)	25,30,33	1.20	2 (8%)
1	CFZ	A	219	1	18,21,22	2.51	7 (38%)	25,30,33	1.50	2 (8%)
1	CFZ	A	328	1	18,21,22	2.55	7 (38%)	25,30,33	1.35	3 (12%)
1	UFT	A	107	1	18,21,22	2.69	10 (55%)	25,30,33	2.08	6 (24%)
1	CFZ	A	271	1	18,21,22	2.51	7 (38%)	25,30,33	1.50	3 (12%)
1	CFZ	A	407	1	18,21,22	2.49	7 (38%)	25,30,33	1.36	3 (12%)
1	CFZ	A	665	1	18,21,22	2.53	7 (38%)	25,30,33	1.49	2 (8%)
1	UFT	A	44	1	18,21,22	2.66	10 (55%)	25,30,33	2.16	7 (28%)
1	UFT	A	643	1	18,21,22	2.62	9 (50%)	25,30,33	1.97	6 (24%)
1	CFZ	A	484	1	18,21,22	2.59	7 (38%)	25,30,33	1.28	1 (4%)
1	CFZ	A	314	1	18,21,22	2.48	7 (38%)	25,30,33	1.38	2 (8%)
1	UFT	A	559	1	18,21,22	2.70	10 (55%)	25,30,33	2.24	7 (28%)
1	CFZ	A	147	1	18,21,22	2.50	7 (38%)	25,30,33	1.43	2 (8%)
1	CFZ	A	80	1	18,21,22	2.52	7 (38%)	25,30,33	1.32	4 (16%)
1	CFZ	A	55	1	18,21,22	2.56	7 (38%)	25,30,33	1.26	2 (8%)
1	UFT	A	88	1	18,21,22	2.60	10 (55%)	25,30,33	2.08	8 (32%)
1	UFT	A	617	1	18,21,22	2.62	10 (55%)	25,30,33	2.10	6 (24%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	UFT	A	46	1	18,21,22	2.69	10 (55%)	25,30,33	1.85	6 (24%)
1	CFZ	A	41	1	18,21,22	2.53	7 (38%)	25,30,33	1.23	2 (8%)
1	UFT	A	504	1	18,21,22	2.68	10 (55%)	25,30,33	2.24	6 (24%)
1	UFT	A	254	1	18,21,22	2.65	10 (55%)	25,30,33	2.00	7 (28%)
1	CFZ	A	645	1	18,21,22	2.48	7 (38%)	25,30,33	1.50	3 (12%)
1	UFT	A	374	1	18,21,22	2.67	10 (55%)	25,30,33	2.16	7 (28%)
1	CFZ	A	522	1	18,21,22	2.53	6 (33%)	25,30,33	1.33	2 (8%)
1	CFZ	A	620	1	18,21,22	2.49	7 (38%)	25,30,33	1.21	2 (8%)
1	UFT	A	79	1	18,21,22	2.61	9 (50%)	25,30,33	2.04	6 (24%)
1	CFZ	A	541	1	18,21,22	2.55	7 (38%)	25,30,33	1.21	1 (4%)
1	CFZ	A	527	1	18,21,22	2.51	7 (38%)	25,30,33	1.54	2 (8%)
1	UFT	A	238	1	18,21,22	2.64	10 (55%)	25,30,33	2.02	8 (32%)
1	UFT	A	71	1	18,21,22	2.67	10 (55%)	25,30,33	2.00	6 (24%)
1	CFZ	A	276	1	18,21,22	2.52	7 (38%)	25,30,33	1.39	2 (8%)
1	UFT	A	507	1	18,21,22	2.68	10 (55%)	25,30,33	1.92	6 (24%)
1	CFZ	A	630	1	18,21,22	2.48	7 (38%)	25,30,33	1.55	2 (8%)
1	UFT	A	644	1	18,21,22	2.63	10 (55%)	25,30,33	2.00	7 (28%)
1	CFZ	A	244	1	18,21,22	2.53	7 (38%)	25,30,33	1.26	3 (12%)
1	UFT	A	582	1	18,21,22	2.65	9 (50%)	25,30,33	1.95	6 (24%)
1	UFT	A	151	1	18,21,22	2.63	9 (50%)	25,30,33	2.02	8 (32%)
1	CFZ	A	217	1	18,21,22	2.56	7 (38%)	25,30,33	1.44	2 (8%)
1	CFZ	A	342	1	18,21,22	2.56	7 (38%)	25,30,33	1.26	2 (8%)
1	UFT	A	33	1	18,21,22	2.66	10 (55%)	25,30,33	2.08	7 (28%)
1	UFT	A	624	1	18,21,22	2.63	10 (55%)	25,30,33	2.04	7 (28%)
1	UFT	A	94	1	18,21,22	2.68	10 (55%)	25,30,33	2.17	7 (28%)
1	UFT	A	468	1	18,21,22	2.58	9 (50%)	25,30,33	1.99	7 (28%)
1	CFZ	A	178	1	18,21,22	2.49	7 (38%)	25,30,33	1.47	3 (12%)
1	CFZ	A	34	1	18,21,22	2.46	6 (33%)	25,30,33	1.27	2 (8%)
1	CFZ	A	204	1	18,21,22	2.51	7 (38%)	25,30,33	1.33	2 (8%)
1	CFZ	A	182	1	18,21,22	2.50	7 (38%)	25,30,33	1.48	3 (12%)
1	CFZ	A	672	1	18,21,22	2.47	7 (38%)	25,30,33	1.16	3 (12%)
1	CFZ	A	287	1	18,21,22	2.53	7 (38%)	25,30,33	1.24	2 (8%)
1	CFZ	A	359	1	18,21,22	2.53	7 (38%)	25,30,33	1.81	6 (24%)
1	CFZ	A	613	1	18,21,22	2.49	6 (33%)	25,30,33	1.37	2 (8%)
1	UFT	A	213	1	18,21,22	2.72	9 (50%)	25,30,33	2.40	8 (32%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CFZ	A	713	1	18,21,22	2.54	6 (33%)	25,30,33	1.77	6 (24%)
1	UFT	A	390	1	18,21,22	2.68	10 (55%)	25,30,33	2.13	6 (24%)
1	UFT	A	705	1	18,21,22	2.62	9 (50%)	25,30,33	1.95	7 (28%)
1	UFT	A	340	1	18,21,22	2.67	10 (55%)	25,30,33	2.01	7 (28%)
1	UFT	A	192	1	18,21,22	2.62	9 (50%)	25,30,33	1.92	6 (24%)
1	CFZ	A	87	1	18,21,22	2.53	7 (38%)	25,30,33	1.30	2 (8%)
1	UFT	A	370	1	18,21,22	2.69	9 (50%)	25,30,33	2.08	6 (24%)
1	CFZ	A	536	1	18,21,22	2.50	7 (38%)	25,30,33	1.27	2 (8%)
1	CFZ	A	561	1	18,21,22	2.51	7 (38%)	25,30,33	1.33	2 (8%)
1	UFT	A	693	1	18,21,22	2.68	10 (55%)	25,30,33	2.09	6 (24%)
1	UFT	A	371	1	18,21,22	2.66	10 (55%)	25,30,33	2.25	8 (32%)
1	UFT	A	383	1	18,21,22	2.64	9 (50%)	25,30,33	1.95	6 (24%)
1	UFT	A	97	1	18,21,22	2.71	9 (50%)	25,30,33	1.94	5 (20%)
1	CFZ	A	591	1	18,21,22	2.45	7 (38%)	25,30,33	1.39	2 (8%)
1	UFT	A	143	1	18,21,22	2.61	10 (55%)	25,30,33	2.05	8 (32%)
1	CFZ	A	344	1	18,21,22	2.53	7 (38%)	25,30,33	1.36	3 (12%)
1	UFT	A	188	1	18,21,22	2.64	9 (50%)	25,30,33	1.92	7 (28%)
1	UFT	A	589	1	18,21,22	2.57	10 (55%)	25,30,33	2.02	7 (28%)
1	CFZ	A	114	1	18,21,22	2.51	7 (38%)	25,30,33	1.41	2 (8%)
1	UFT	A	17	1	18,21,22	2.64	9 (50%)	25,30,33	1.98	7 (28%)
1	UFT	A	562	1	18,21,22	2.60	9 (50%)	25,30,33	2.11	8 (32%)
1	UFT	A	501	1	18,21,22	2.61	9 (50%)	25,30,33	1.93	7 (28%)
1	CFZ	A	422	1	18,21,22	2.54	7 (38%)	25,30,33	1.25	2 (8%)
1	UFT	A	32	1	18,21,22	2.62	10 (55%)	25,30,33	2.06	8 (32%)
1	UFT	A	181	1	18,21,22	2.57	9 (50%)	25,30,33	1.87	7 (28%)
1	CFZ	A	291	1	18,21,22	2.52	7 (38%)	25,30,33	1.27	3 (12%)
1	CFZ	A	547	1	18,21,22	2.47	7 (38%)	25,30,33	1.43	2 (8%)
1	CFZ	A	490	1	18,21,22	2.55	7 (38%)	25,30,33	1.22	3 (12%)
1	CFZ	A	653	1	18,21,22	2.49	7 (38%)	25,30,33	1.21	2 (8%)
1	CFZ	A	499	1	18,21,22	2.52	7 (38%)	25,30,33	1.58	2 (8%)
1	UFT	A	523	1	18,21,22	2.61	9 (50%)	25,30,33	1.94	6 (24%)
1	CFZ	A	171	1	18,21,22	2.46	7 (38%)	25,30,33	1.51	2 (8%)
1	UFT	A	267	1	18,21,22	2.66	10 (55%)	25,30,33	2.15	7 (28%)
1	CFZ	A	463	1	18,21,22	2.54	8 (44%)	25,30,33	1.58	4 (16%)
1	CFZ	A	256	1	18,21,22	2.51	7 (38%)	25,30,33	1.59	3 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CFZ	A	493	1	18,21,22	2.52	7 (38%)	25,30,33	1.33	2 (8%)
1	CFZ	A	173	1	18,21,22	2.50	6 (33%)	25,30,33	1.13	2 (8%)
1	UFT	A	616	1	18,21,22	2.62	10 (55%)	25,30,33	2.06	8 (32%)
1	CFZ	A	663	1	18,21,22	2.50	7 (38%)	25,30,33	1.38	4 (16%)
1	UFT	A	638	1	18,21,22	2.66	10 (55%)	25,30,33	2.24	8 (32%)
1	UFT	A	549	1	18,21,22	2.65	10 (55%)	25,30,33	1.90	7 (28%)
1	UFT	A	58	1	18,21,22	2.60	10 (55%)	25,30,33	2.31	7 (28%)
1	CFZ	A	135	1	18,21,22	2.55	7 (38%)	25,30,33	1.28	2 (8%)
1	CFZ	A	689	1	18,21,22	2.52	7 (38%)	25,30,33	1.25	2 (8%)
1	CFZ	A	81	1	18,21,22	2.50	7 (38%)	25,30,33	1.32	2 (8%)
1	UFT	A	339	1	18,21,22	2.69	9 (50%)	25,30,33	2.06	7 (28%)
1	CFZ	A	635	1	18,21,22	2.54	7 (38%)	25,30,33	1.32	3 (12%)
1	UFT	A	120	1	18,21,22	2.63	10 (55%)	25,30,33	2.20	7 (28%)
1	UFT	A	697	1	18,21,22	2.60	9 (50%)	25,30,33	2.06	8 (32%)
1	UFT	A	322	1	18,21,22	2.59	10 (55%)	25,30,33	2.14	9 (36%)
1	UFT	A	429	1	18,21,22	2.72	9 (50%)	25,30,33	1.89	7 (28%)
1	CFZ	A	269	1	18,21,22	2.46	7 (38%)	25,30,33	1.38	3 (12%)
1	UFT	A	431	1	18,21,22	2.64	9 (50%)	25,30,33	2.13	7 (28%)
1	CFZ	A	694	1	18,21,22	2.51	7 (38%)	25,30,33	1.28	2 (8%)
1	CFZ	A	362	1	18,21,22	2.50	7 (38%)	25,30,33	1.50	5 (20%)
1	UFT	A	558	1	18,21,22	2.66	10 (55%)	25,30,33	2.08	7 (28%)
1	UFT	A	716	1	18,21,22	2.66	10 (55%)	25,30,33	2.06	6 (24%)
1	UFT	A	686	1	18,21,22	2.65	9 (50%)	25,30,33	2.06	9 (36%)
1	CFZ	A	458	1	18,21,22	2.52	7 (38%)	25,30,33	1.28	3 (12%)
1	CFZ	A	706	1	18,21,22	2.47	6 (33%)	25,30,33	1.31	2 (8%)
1	UFT	A	42	1	18,21,22	2.66	10 (55%)	25,30,33	1.97	6 (24%)
1	UFT	A	19	1	18,21,22	2.66	10 (55%)	25,30,33	2.00	6 (24%)
1	CFZ	A	336	1	18,21,22	2.55	7 (38%)	25,30,33	1.40	2 (8%)
1	UFT	A	588	1	18,21,22	2.57	10 (55%)	25,30,33	2.17	8 (32%)
1	CFZ	A	146	1	18,21,22	2.43	7 (38%)	25,30,33	1.33	3 (12%)
1	UFT	A	277	1	18,21,22	2.61	10 (55%)	25,30,33	2.25	7 (28%)
1	CFZ	A	720	1	18,21,22	2.47	7 (38%)	25,30,33	1.42	3 (12%)
1	CFZ	A	198	1	18,21,22	2.56	7 (38%)	25,30,33	1.24	2 (8%)
1	UFT	A	303	1	18,21,22	2.64	10 (55%)	25,30,33	2.20	7 (28%)
1	UFT	A	655	1	18,21,22	2.61	9 (50%)	25,30,33	2.03	7 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	UFT	A	148	1	18,21,22	2.69	10 (55%)	25,30,33	1.89	6 (24%)
1	CFZ	A	65	1	18,21,22	2.48	7 (38%)	25,30,33	1.42	3 (12%)
1	UFT	A	230	1	18,21,22	2.66	10 (55%)	25,30,33	2.06	5 (20%)
1	CFZ	A	560	1	18,21,22	2.51	7 (38%)	25,30,33	1.24	2 (8%)
1	CFZ	A	73	1	18,21,22	2.44	7 (38%)	25,30,33	1.55	2 (8%)
1	CFZ	A	83	1	18,21,22	2.60	7 (38%)	25,30,33	1.25	2 (8%)
1	CFZ	A	546	1	18,21,22	2.53	7 (38%)	25,30,33	1.22	1 (4%)
1	UFT	A	550	1	18,21,22	2.67	10 (55%)	25,30,33	2.19	8 (32%)
1	CFZ	A	10	1	18,21,22	2.54	7 (38%)	25,30,33	1.33	2 (8%)
1	UFT	A	6	1	18,21,22	2.65	10 (55%)	25,30,33	1.97	6 (24%)
1	CFZ	A	131	1	18,21,22	2.48	7 (38%)	25,30,33	1.55	3 (12%)

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	CFZ	A	161	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	11	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	485	1	-	0/7/25/26	0/2/2/2
1	UFT	A	409	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	717	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	426	1	-	0/7/25/26	0/2/2/2
1	UFT	A	542	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	632	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	661	1	-	2/7/25/26	0/2/2/2
1	UFT	A	595	1	-	1/7/25/26	0/2/2/2
1	UFT	A	627	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	405	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	346	1	-	1/7/25/26	0/2/2/2
1	UFT	A	670	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	128	1	-	7/7/25/26	0/2/2/2
1	UFT	A	236	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	658	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	206	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	275	1	-	0/7/25/26	0/2/2/2
1	UFT	A	61	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	51	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	577	1	-	0/7/25/26	0/2/2/2
1	UFT	A	95	1	-	0/7/25/26	0/2/2/2
1	UFT	A	283	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	518	1	-	0/7/25/26	0/2/2/2
1	UFT	A	471	1	-	0/7/25/26	0/2/2/2
1	UFT	A	329	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	45	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	72	1	-	4/7/25/26	0/2/2/2
1	UFT	A	196	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	675	1	-	3/7/25/26	0/2/2/2
1	UFT	A	175	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	63	1	-	0/7/25/26	0/2/2/2
1	UFT	A	475	1	-	3/7/25/26	0/2/2/2
1	UFT	A	667	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	50	1	-	0/7/25/26	0/2/2/2
1	UFT	A	585	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	165	1	-	0/7/25/26	0/2/2/2
1	UFT	A	56	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	433	1	-	0/7/25/26	0/2/2/2
1	UFT	A	575	1	-	4/7/25/26	0/2/2/2
1	UFT	A	444	1	-	0/7/25/26	0/2/2/2
1	UFT	A	650	1	-	2/7/25/26	0/2/2/2
1	UFT	A	115	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	195	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	75	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	602	1	-	2/7/25/26	0/2/2/2
1	UFT	A	683	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	137	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	500	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	416	1	-	0/7/25/26	0/2/2/2
1	UFT	A	607	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	101	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	184	1	-	0/7/25/26	0/2/2/2
1	UFT	A	298	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	460	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	578	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	233	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	355	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	442	1	-	0/7/25/26	0/2/2/2
1	UFT	A	193	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	308	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	609	1	-	0/7/25/26	0/2/2/2
1	UFT	A	62	1	-	3/7/25/26	0/2/2/2
1	UFT	A	311	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	649	1	-	2/7/25/26	0/2/2/2
1	UFT	A	464	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	337	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	618	1	-	2/7/25/26	0/2/2/2
1	UFT	A	221	1	-	3/7/25/26	0/2/2/2
1	UFT	A	727	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	57	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	621	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	392	1	-	0/7/25/26	0/2/2/2
1	UFT	A	274	1	-	3/7/25/26	0/2/2/2
1	UFT	A	679	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	637	1	-	0/7/25/26	0/2/2/2
1	UFT	A	93	1	-	0/7/25/26	0/2/2/2
1	UFT	A	194	1	-	0/7/25/26	0/2/2/2
1	UFT	A	154	1	-	1/7/25/26	0/2/2/2
1	UFT	A	215	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	144	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	382	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	162	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	90	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	129	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	111	1	-	0/7/25/26	0/2/2/2
1	UFT	A	556	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	506	1	-	0/7/25/26	0/2/2/2
1	UFT	A	138	1	-	0/7/25/26	0/2/2/2
1	UFT	A	127	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	332	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	391	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	15	1	-	0/7/25/26	0/2/2/2
1	UFT	A	724	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	656	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	153	1	-	0/7/25/26	0/2/2/2
1	UFT	A	48	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	483	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	438	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	515	1	-	2/7/25/26	0/2/2/2
1	UFT	A	388	1	-	0/7/25/26	0/2/2/2
1	UFT	A	698	1	-	0/7/25/26	0/2/2/2
1	UFT	A	116	1	-	2/7/25/26	0/2/2/2
1	UFT	A	169	1	-	0/7/25/26	0/2/2/2
1	UFT	A	360	1	-	3/7/25/26	0/2/2/2
1	UFT	A	123	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	526	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	208	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	641	1	-	0/7/25/26	0/2/2/2
1	UFT	A	451	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	690	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	121	1	-	0/7/25/26	0/2/2/2
1	UFT	A	345	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	108	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	456	1	-	0/7/25/26	0/2/2/2
1	UFT	A	417	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	330	1	-	2/7/25/26	0/2/2/2
1	UFT	A	361	1	-	0/7/25/26	0/2/2/2
1	UFT	A	350	1	-	0/7/25/26	0/2/2/2
1	UFT	A	319	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	502	1	-	3/7/25/26	0/2/2/2
1	UFT	A	573	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	625	1	-	0/7/25/26	0/2/2/2
1	UFT	A	240	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	466	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	603	1	-	2/7/25/26	0/2/2/2
1	UFT	A	555	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	190	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	384	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	452	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	657	1	-	6/7/25/26	0/2/2/2
1	CFZ	A	473	1	-	0/7/25/26	0/2/2/2
1	UFT	A	612	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	674	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	103	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	557	1	-	1/7/25/26	0/2/2/2
1	UFT	A	307	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	709	1	-	4/7/25/26	0/2/2/2
1	CFZ	A	273	1	-	1/7/25/26	0/2/2/2
1	UFT	A	532	1	-	0/7/25/26	0/2/2/2
1	UFT	A	497	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	538	1	-	0/7/25/26	0/2/2/2
1	UFT	A	601	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	28	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	629	1	-	0/7/25/26	0/2/2/2
1	UFT	A	167	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	695	1	-	0/7/25/26	0/2/2/2
1	UFT	A	177	1	-	1/7/25/26	0/2/2/2
1	UFT	A	23	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	209	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	156	1	-	0/7/25/26	0/2/2/2
1	UFT	A	642	1	-	1/7/25/26	0/2/2/2
1	UFT	A	170	1	-	0/7/25/26	0/2/2/2
1	UFT	A	671	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	104	1	-	0/7/25/26	0/2/2/2
1	UFT	A	397	1	-	1/7/25/26	0/2/2/2
1	UFT	A	510	1	-	1/7/25/26	0/2/2/2
1	UFT	A	89	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	594	1	-	0/7/25/26	0/2/2/2
1	UFT	A	419	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	335	1	-	1/7/25/26	0/2/2/2
1	UFT	A	197	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	379	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	685	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	12	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	306	1	-	0/7/25/26	0/2/2/2
1	UFT	A	39	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	363	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	467	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	366	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	696	1	-	2/7/25/26	0/2/2/2
1	UFT	A	263	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	310	1	-	0/7/25/26	0/2/2/2
1	UFT	A	476	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	590	1	-	2/7/25/26	0/2/2/2
1	UFT	A	272	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	157	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	395	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	7	1	-	0/7/25/26	0/2/2/2
1	UFT	A	597	1	-	0/7/25/26	0/2/2/2
1	UFT	A	521	1	-	2/7/25/26	0/2/2/2
1	UFT	A	351	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	487	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	598	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	631	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	434	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	212	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	155	1	-	0/7/25/26	0/2/2/2
1	UFT	A	480	1	-	0/7/25/26	0/2/2/2
1	UFT	A	242	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	531	1	-	2/7/25/26	0/2/2/2
1	UFT	A	662	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	302	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	369	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	26	1	-	0/7/25/26	0/2/2/2
1	UFT	A	377	1	-	6/7/25/26	0/2/2/2
1	CFZ	A	234	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	343	1	-	0/7/25/26	0/2/2/2
1	UFT	A	356	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	564	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	76	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	574	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	699	1	-	0/7/25/26	0/2/2/2
1	UFT	A	563	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	130	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	432	1	-	0/7/25/26	0/2/2/2
1	UFT	A	421	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	666	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	117	1	-	0/7/25/26	0/2/2/2
1	UFT	A	367	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	437	1	-	0/7/25/26	0/2/2/2
1	UFT	A	66	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	109	1	-	0/7/25/26	0/2/2/2
1	UFT	A	210	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	288	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	489	1	-	0/7/25/26	0/2/2/2
1	UFT	A	142	1	-	3/7/25/26	0/2/2/2
1	UFT	A	719	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	512	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	453	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	386	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	600	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	728	1	-	5/7/25/26	0/2/2/2
1	CFZ	A	605	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	219	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	328	1	-	0/7/25/26	0/2/2/2
1	UFT	A	107	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	271	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	407	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	665	1	-	0/7/25/26	0/2/2/2
1	UFT	A	44	1	-	1/7/25/26	0/2/2/2
1	UFT	A	643	1	-	4/7/25/26	0/2/2/2
1	CFZ	A	484	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	314	1	-	0/7/25/26	0/2/2/2
1	UFT	A	559	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	147	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	80	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	55	1	-	2/7/25/26	0/2/2/2
1	UFT	A	88	1	-	3/7/25/26	0/2/2/2
1	UFT	A	617	1	-	3/7/25/26	0/2/2/2
1	UFT	A	46	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	41	1	-	0/7/25/26	0/2/2/2
1	UFT	A	504	1	-	3/7/25/26	0/2/2/2
1	UFT	A	254	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	645	1	-	2/7/25/26	0/2/2/2
1	UFT	A	374	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	522	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	620	1	-	0/7/25/26	0/2/2/2
1	UFT	A	79	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	541	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	527	1	-	2/7/25/26	0/2/2/2
1	UFT	A	238	1	-	0/7/25/26	0/2/2/2
1	UFT	A	71	1	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CFZ	A	276	1	-	0/7/25/26	0/2/2/2
1	UFT	A	507	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	630	1	-	0/7/25/26	0/2/2/2
1	UFT	A	644	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	244	1	-	2/7/25/26	0/2/2/2
1	UFT	A	582	1	-	0/7/25/26	0/2/2/2
1	UFT	A	151	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	217	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	342	1	-	0/7/25/26	0/2/2/2
1	UFT	A	33	1	-	2/7/25/26	0/2/2/2
1	UFT	A	624	1	-	0/7/25/26	0/2/2/2
1	UFT	A	94	1	-	3/7/25/26	0/2/2/2
1	UFT	A	468	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	178	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	34	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	204	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	182	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	672	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	287	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	359	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	613	1	-	0/7/25/26	0/2/2/2
1	UFT	A	213	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	713	1	-	3/7/25/26	0/2/2/2
1	UFT	A	390	1	-	0/7/25/26	0/2/2/2
1	UFT	A	705	1	-	0/7/25/26	0/2/2/2
1	UFT	A	340	1	-	0/7/25/26	0/2/2/2
1	UFT	A	192	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	87	1	-	0/7/25/26	0/2/2/2
1	UFT	A	370	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	536	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	561	1	-	0/7/25/26	0/2/2/2
1	UFT	A	693	1	-	0/7/25/26	0/2/2/2
1	UFT	A	371	1	-	2/7/25/26	0/2/2/2
1	UFT	A	383	1	-	0/7/25/26	0/2/2/2
1	UFT	A	97	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	591	1	-	3/7/25/26	0/2/2/2
1	UFT	A	143	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	344	1	-	0/7/25/26	0/2/2/2
1	UFT	A	188	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	589	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	114	1	-	2/7/25/26	0/2/2/2
1	UFT	A	17	1	-	2/7/25/26	0/2/2/2
1	UFT	A	562	1	-	0/7/25/26	0/2/2/2
1	UFT	A	501	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	422	1	-	0/7/25/26	0/2/2/2
1	UFT	A	32	1	-	2/7/25/26	0/2/2/2
1	UFT	A	181	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	291	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	547	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	490	1	-	3/7/25/26	0/2/2/2
1	CFZ	A	653	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	499	1	-	2/7/25/26	0/2/2/2
1	UFT	A	523	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	171	1	-	2/7/25/26	0/2/2/2
1	UFT	A	267	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	463	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	256	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	493	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	173	1	-	0/7/25/26	0/2/2/2
1	UFT	A	616	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	663	1	-	0/7/25/26	0/2/2/2
1	UFT	A	638	1	-	0/7/25/26	0/2/2/2
1	UFT	A	549	1	-	0/7/25/26	0/2/2/2
1	UFT	A	58	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	135	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	689	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	81	1	-	0/7/25/26	0/2/2/2
1	UFT	A	339	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	635	1	-	0/7/25/26	0/2/2/2
1	UFT	A	120	1	-	1/7/25/26	0/2/2/2
1	UFT	A	697	1	-	1/7/25/26	0/2/2/2
1	UFT	A	322	1	-	2/7/25/26	0/2/2/2
1	UFT	A	429	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	269	1	-	0/7/25/26	0/2/2/2
1	UFT	A	431	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	694	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	362	1	-	2/7/25/26	0/2/2/2
1	UFT	A	558	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UFT	A	716	1	-	2/7/25/26	0/2/2/2
1	UFT	A	686	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	458	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	706	1	-	0/7/25/26	0/2/2/2
1	UFT	A	42	1	-	0/7/25/26	0/2/2/2
1	UFT	A	19	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	336	1	-	1/7/25/26	0/2/2/2
1	UFT	A	588	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	146	1	-	1/7/25/26	0/2/2/2
1	UFT	A	277	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	720	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	198	1	-	2/7/25/26	0/2/2/2
1	UFT	A	303	1	-	1/7/25/26	0/2/2/2
1	UFT	A	655	1	-	3/7/25/26	0/2/2/2
1	UFT	A	148	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	65	1	-	0/7/25/26	0/2/2/2
1	UFT	A	230	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	560	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	73	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	83	1	-	0/7/25/26	0/2/2/2
1	CFZ	A	546	1	-	0/7/25/26	0/2/2/2
1	UFT	A	550	1	-	2/7/25/26	0/2/2/2
1	CFZ	A	10	1	-	0/7/25/26	0/2/2/2
1	UFT	A	6	1	-	1/7/25/26	0/2/2/2
1	CFZ	A	131	1	-	1/7/25/26	0/2/2/2

All (2919) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	573	UFT	C2-N1	5.43	1.47	1.38
1	A	23	UFT	C2-N1	5.38	1.46	1.38
1	A	194	UFT	C2-N1	5.36	1.46	1.38
1	A	71	UFT	C2-N1	5.34	1.46	1.38
1	A	429	UFT	C2-N1	5.33	1.46	1.38
1	A	94	UFT	C2-N1	5.27	1.46	1.38
1	A	475	UFT	C2-N1	5.26	1.46	1.38
1	A	339	UFT	C2-N1	5.24	1.46	1.38
1	A	48	UFT	C2-N1	5.21	1.46	1.38
1	A	419	UFT	C2-N1	5.21	1.46	1.38
1	A	93	UFT	C2-N1	5.20	1.46	1.38
1	A	727	UFT	C2-N1	5.20	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	UFT	C2-N1	5.19	1.46	1.38
1	A	148	UFT	C2-N1	5.16	1.46	1.38
1	A	360	UFT	C2-N1	5.16	1.46	1.38
1	A	213	UFT	C2-N1	5.16	1.46	1.38
1	A	409	UFT	C2-N1	5.14	1.46	1.38
1	A	46	UFT	C2-N1	5.13	1.46	1.38
1	A	210	UFT	C2-N1	5.12	1.46	1.38
1	A	215	UFT	C2-N1	5.12	1.46	1.38
1	A	559	UFT	C2-N1	5.12	1.46	1.38
1	A	497	UFT	C2-N1	5.11	1.46	1.38
1	A	177	UFT	C2-N1	5.11	1.46	1.38
1	A	56	UFT	C2-N1	5.10	1.46	1.38
1	A	370	UFT	C2-N1	5.10	1.46	1.38
1	A	390	UFT	C2-N1	5.08	1.46	1.38
1	A	221	UFT	C2-N1	5.08	1.46	1.38
1	A	504	UFT	C2-N1	5.07	1.46	1.38
1	A	367	UFT	C2-N1	5.07	1.46	1.38
1	A	188	UFT	C2-N1	5.06	1.46	1.38
1	A	120	UFT	C2-N1	5.06	1.46	1.38
1	A	650	UFT	C2-N1	5.05	1.46	1.38
1	A	643	UFT	C2-N1	5.04	1.46	1.38
1	A	97	UFT	C2-N1	5.04	1.46	1.38
1	A	631	CFZ	C2'-C3'	-5.04	1.46	1.52
1	A	549	UFT	C2-N1	5.03	1.46	1.38
1	A	307	UFT	C2-N1	5.03	1.46	1.38
1	A	601	UFT	C2-N1	5.02	1.46	1.38
1	A	169	UFT	C2-N1	5.01	1.46	1.38
1	A	175	UFT	C2-N1	5.00	1.46	1.38
1	A	371	UFT	C2-N1	5.00	1.46	1.38
1	A	388	UFT	C2-N1	4.99	1.46	1.38
1	A	55	CFZ	C2'-C3'	-4.99	1.46	1.52
1	A	17	UFT	C2-N1	4.99	1.46	1.38
1	A	471	UFT	C2-N1	4.99	1.46	1.38
1	A	39	UFT	C2-N1	4.99	1.46	1.38
1	A	612	UFT	C2-N1	4.99	1.46	1.38
1	A	66	UFT	C2-N1	4.98	1.46	1.38
1	A	638	UFT	C2-N1	4.98	1.46	1.38
1	A	550	UFT	C2-N1	4.98	1.46	1.38
1	A	274	UFT	C2-N1	4.97	1.46	1.38
1	A	123	UFT	C2-N1	4.97	1.46	1.38
1	A	671	UFT	C2-N1	4.97	1.46	1.38
1	A	377	UFT	C2'-C3'	-4.97	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	555	UFT	C2-N1	4.96	1.46	1.38
1	A	44	UFT	C2-N1	4.96	1.46	1.38
1	A	267	UFT	C2-N1	4.96	1.46	1.38
1	A	578	CFZ	C2'-C3'	-4.95	1.46	1.52
1	A	523	UFT	C2-N1	4.95	1.46	1.38
1	A	507	UFT	C2-N1	4.95	1.46	1.38
1	A	308	CFZ	C2'-C3'	-4.95	1.46	1.52
1	A	283	UFT	C2-N1	4.94	1.46	1.38
1	A	716	UFT	C2-N1	4.94	1.46	1.38
1	A	627	UFT	C2-N1	4.94	1.46	1.38
1	A	230	UFT	C2-N1	4.93	1.46	1.38
1	A	719	UFT	C2-N1	4.93	1.46	1.38
1	A	116	UFT	C2-N1	4.92	1.46	1.38
1	A	674	CFZ	C4-N4	4.91	1.45	1.33
1	A	617	UFT	C2-N1	4.91	1.46	1.38
1	A	263	UFT	C2-N1	4.90	1.46	1.38
1	A	679	UFT	C2-N1	4.90	1.46	1.38
1	A	236	UFT	C2-N1	4.90	1.46	1.38
1	A	198	CFZ	C2'-C3'	-4.89	1.46	1.52
1	A	713	CFZ	C4-N4	4.89	1.45	1.33
1	A	693	UFT	C2-N1	4.89	1.46	1.38
1	A	65	CFZ	C4-N4	4.88	1.45	1.33
1	A	51	UFT	C2-N1	4.88	1.46	1.38
1	A	468	UFT	C2-N1	4.88	1.46	1.38
1	A	170	UFT	C2-N1	4.88	1.46	1.38
1	A	356	UFT	C2-N1	4.88	1.46	1.38
1	A	303	UFT	C2-N1	4.87	1.46	1.38
1	A	361	UFT	C2-N1	4.87	1.46	1.38
1	A	431	UFT	C2-N1	4.87	1.46	1.38
1	A	288	UFT	C2-N1	4.87	1.46	1.38
1	A	33	UFT	C2-N1	4.87	1.46	1.38
1	A	538	CFZ	C2'-C3'	-4.87	1.46	1.52
1	A	277	UFT	C2-N1	4.87	1.46	1.38
1	A	374	UFT	C2-N1	4.86	1.46	1.38
1	A	556	UFT	C2-N1	4.86	1.46	1.38
1	A	687	UFT	C2-N1	4.86	1.46	1.38
1	A	171	CFZ	C4-N4	4.86	1.45	1.33
1	A	578	CFZ	C4-N4	4.86	1.45	1.33
1	A	135	CFZ	C2'-C3'	-4.86	1.46	1.52
1	A	350	UFT	C2-N1	4.86	1.46	1.38
1	A	460	CFZ	C4-N4	4.86	1.45	1.33
1	A	117	CFZ	C4-N4	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	CFZ	C4-N4	4.85	1.45	1.33
1	A	319	UFT	C2-N1	4.85	1.46	1.38
1	A	490	CFZ	C4-N4	4.85	1.45	1.33
1	A	595	UFT	C2-N1	4.84	1.46	1.38
1	A	538	CFZ	C4-N4	4.84	1.45	1.33
1	A	369	CFZ	C4-N4	4.84	1.45	1.33
1	A	28	CFZ	C4-N4	4.84	1.45	1.33
1	A	302	CFZ	C4-N4	4.84	1.45	1.33
1	A	76	CFZ	C2'-C3'	-4.84	1.46	1.52
1	A	485	UFT	C2-N1	4.83	1.46	1.38
1	A	7	CFZ	C2'-C3'	-4.83	1.46	1.52
1	A	451	UFT	C2-N1	4.83	1.46	1.38
1	A	12	CFZ	C4-N4	4.83	1.45	1.33
1	A	144	CFZ	C4-N4	4.83	1.45	1.33
1	A	328	CFZ	C2'-C3'	-4.83	1.46	1.52
1	A	575	UFT	C2-N1	4.83	1.46	1.38
1	A	298	UFT	C2-N1	4.82	1.46	1.38
1	A	165	CFZ	C4-N4	4.82	1.45	1.33
1	A	686	UFT	C2-N1	4.82	1.46	1.38
1	A	208	CFZ	C4-N4	4.82	1.45	1.33
1	A	699	CFZ	C4-N4	4.82	1.45	1.33
1	A	536	CFZ	C4-N4	4.82	1.45	1.33
1	A	198	CFZ	C4-N4	4.82	1.45	1.33
1	A	655	UFT	C2-N1	4.82	1.46	1.38
1	A	392	CFZ	C4-N4	4.82	1.45	1.33
1	A	591	CFZ	C4-N4	4.82	1.45	1.33
1	A	493	CFZ	C4-N4	4.82	1.45	1.33
1	A	502	CFZ	C4-N4	4.81	1.45	1.33
1	A	422	CFZ	C2'-C3'	-4.81	1.46	1.52
1	A	635	CFZ	C4-N4	4.81	1.45	1.33
1	A	55	CFZ	C4-N4	4.81	1.45	1.33
1	A	19	UFT	C2-N1	4.81	1.46	1.38
1	A	87	CFZ	C4-N4	4.80	1.45	1.33
1	A	564	CFZ	C4-N4	4.80	1.45	1.33
1	A	597	UFT	C2-N1	4.80	1.46	1.38
1	A	306	CFZ	C2'-C3'	-4.80	1.46	1.52
1	A	464	UFT	C2-N1	4.80	1.46	1.38
1	A	271	CFZ	C4-N4	4.80	1.45	1.33
1	A	487	CFZ	C2'-C3'	-4.80	1.46	1.52
1	A	238	UFT	C2-N1	4.80	1.46	1.38
1	A	121	CFZ	C4-N4	4.80	1.45	1.33
1	A	490	CFZ	C2'-C3'	-4.80	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	CFZ	C2'-C3'	-4.80	1.46	1.52
1	A	656	CFZ	C4-N4	4.80	1.45	1.33
1	A	672	CFZ	C4-N4	4.80	1.45	1.33
1	A	234	CFZ	C2'-C3'	-4.80	1.46	1.52
1	A	233	CFZ	C4-N4	4.80	1.45	1.33
1	A	618	CFZ	C4-N4	4.80	1.45	1.33
1	A	83	CFZ	C4-N4	4.80	1.45	1.33
1	A	90	CFZ	C4-N4	4.80	1.45	1.33
1	A	421	UFT	C2-N1	4.79	1.46	1.38
1	A	602	CFZ	C4-N4	4.79	1.45	1.33
1	A	212	CFZ	C4-N4	4.79	1.45	1.33
1	A	542	UFT	C2-N1	4.79	1.46	1.38
1	A	287	CFZ	C4-N4	4.79	1.45	1.33
1	A	62	UFT	C2-N1	4.79	1.46	1.38
1	A	254	UFT	C2-N1	4.79	1.46	1.38
1	A	197	UFT	C2-N1	4.79	1.46	1.38
1	A	80	CFZ	C4-N4	4.79	1.45	1.33
1	A	632	CFZ	C4-N4	4.79	1.45	1.33
1	A	605	CFZ	C2'-C3'	-4.79	1.46	1.52
1	A	63	CFZ	C4-N4	4.79	1.45	1.33
1	A	156	CFZ	C2'-C3'	-4.79	1.46	1.52
1	A	81	CFZ	C4-N4	4.79	1.45	1.33
1	A	244	CFZ	C4-N4	4.79	1.45	1.33
1	A	697	UFT	C2-N1	4.78	1.46	1.38
1	A	645	CFZ	C4-N4	4.78	1.45	1.33
1	A	155	CFZ	C4-N4	4.78	1.45	1.33
1	A	386	CFZ	C4-N4	4.78	1.45	1.33
1	A	541	CFZ	C2'-C3'	-4.78	1.46	1.52
1	A	57	CFZ	C4-N4	4.78	1.45	1.33
1	A	7	CFZ	C4-N4	4.78	1.45	1.33
1	A	26	CFZ	C4-N4	4.78	1.45	1.33
1	A	337	CFZ	C4-N4	4.78	1.45	1.33
1	A	695	CFZ	C4-N4	4.78	1.45	1.33
1	A	456	CFZ	C4-N4	4.78	1.45	1.33
1	A	662	UFT	C2-N1	4.78	1.45	1.38
1	A	346	CFZ	C4-N4	4.78	1.45	1.33
1	A	590	UFT	C2-N1	4.78	1.45	1.38
1	A	366	CFZ	C4-N4	4.78	1.45	1.33
1	A	405	CFZ	C4-N4	4.78	1.45	1.33
1	A	642	UFT	C2-N1	4.78	1.45	1.38
1	A	114	CFZ	C4-N4	4.78	1.45	1.33
1	A	153	CFZ	C4-N4	4.78	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	561	CFZ	C4-N4	4.78	1.45	1.33
1	A	605	CFZ	C4-N4	4.78	1.45	1.33
1	A	15	CFZ	C4-N4	4.78	1.45	1.33
1	A	603	CFZ	C4-N4	4.77	1.45	1.33
1	A	661	CFZ	C4-N4	4.77	1.45	1.33
1	A	330	CFZ	C4-N4	4.77	1.45	1.33
1	A	463	CFZ	C4-N4	4.77	1.45	1.33
1	A	45	CFZ	C4-N4	4.77	1.45	1.33
1	A	310	CFZ	C4-N4	4.77	1.45	1.33
1	A	107	UFT	C2-N1	4.77	1.45	1.38
1	A	621	CFZ	C4-N4	4.77	1.45	1.33
1	A	131	CFZ	C4-N4	4.77	1.45	1.33
1	A	484	CFZ	C4-N4	4.77	1.45	1.33
1	A	72	CFZ	C4-N4	4.77	1.45	1.33
1	A	466	CFZ	C4-N4	4.77	1.45	1.33
1	A	362	CFZ	C4-N4	4.77	1.45	1.33
1	A	104	CFZ	C2'-C3'	-4.77	1.46	1.52
1	A	127	UFT	C2-N1	4.77	1.45	1.38
1	A	467	CFZ	C4-N4	4.76	1.45	1.33
1	A	716	UFT	C6-N1	4.76	1.49	1.38
1	A	438	CFZ	C4-N4	4.76	1.45	1.33
1	A	182	CFZ	C4-N4	4.76	1.45	1.33
1	A	473	CFZ	C4-N4	4.76	1.45	1.33
1	A	452	CFZ	C2'-C3'	-4.76	1.46	1.52
1	A	426	CFZ	C4-N4	4.76	1.45	1.33
1	A	483	CFZ	C4-N4	4.76	1.45	1.33
1	A	658	CFZ	C4-N4	4.76	1.45	1.33
1	A	340	UFT	C2-N1	4.76	1.45	1.38
1	A	527	CFZ	C4-N4	4.76	1.45	1.33
1	A	391	CFZ	C4-N4	4.76	1.45	1.33
1	A	558	UFT	C2-N1	4.76	1.45	1.38
1	A	641	CFZ	C4-N4	4.76	1.45	1.33
1	A	193	UFT	C2-N1	4.76	1.45	1.38
1	A	407	CFZ	C4-N4	4.76	1.45	1.33
1	A	129	CFZ	C4-N4	4.75	1.45	1.33
1	A	42	UFT	C2-N1	4.75	1.45	1.38
1	A	487	CFZ	C4-N4	4.75	1.45	1.33
1	A	574	CFZ	C4-N4	4.75	1.45	1.33
1	A	57	CFZ	C2'-C3'	-4.75	1.46	1.52
1	A	442	CFZ	C4-N4	4.75	1.45	1.33
1	A	10	CFZ	C4-N4	4.75	1.45	1.33
1	A	291	CFZ	C4-N4	4.75	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	463	CFZ	C2'-C3'	-4.75	1.46	1.52
1	A	156	CFZ	C4-N4	4.75	1.45	1.33
1	A	240	UFT	C2-N1	4.75	1.45	1.38
1	A	384	CFZ	C2'-C3'	-4.75	1.46	1.52
1	A	206	CFZ	C4-N4	4.75	1.45	1.33
1	A	161	CFZ	C4-N4	4.75	1.45	1.33
1	A	609	CFZ	C4-N4	4.75	1.45	1.33
1	A	95	UFT	C2-N1	4.75	1.45	1.38
1	A	694	CFZ	C2'-C3'	-4.75	1.46	1.52
1	A	499	CFZ	C4-N4	4.75	1.45	1.33
1	A	500	CFZ	C4-N4	4.75	1.45	1.33
1	A	384	CFZ	C4-N4	4.75	1.45	1.33
1	A	151	UFT	C2-N1	4.75	1.45	1.38
1	A	613	CFZ	C4-N4	4.75	1.45	1.33
1	A	452	CFZ	C4-N4	4.75	1.45	1.33
1	A	696	CFZ	C2'-C3'	-4.75	1.46	1.52
1	A	546	CFZ	C2'-C3'	-4.74	1.46	1.52
1	A	108	CFZ	C4-N4	4.74	1.45	1.33
1	A	209	CFZ	C4-N4	4.74	1.45	1.33
1	A	598	CFZ	C4-N4	4.74	1.45	1.33
1	A	73	CFZ	C4-N4	4.74	1.45	1.33
1	A	594	CFZ	C4-N4	4.74	1.45	1.33
1	A	631	CFZ	C4-N4	4.74	1.45	1.33
1	A	104	CFZ	C4-N4	4.74	1.45	1.33
1	A	720	CFZ	C4-N4	4.74	1.45	1.33
1	A	342	CFZ	C2'-C3'	-4.74	1.46	1.52
1	A	344	CFZ	C4-N4	4.74	1.45	1.33
1	A	689	CFZ	C4-N4	4.74	1.45	1.33
1	A	453	CFZ	C4-N4	4.74	1.45	1.33
1	A	137	CFZ	C4-N4	4.74	1.45	1.33
1	A	329	UFT	C2-N1	4.74	1.45	1.38
1	A	76	CFZ	C4-N4	4.74	1.45	1.33
1	A	195	CFZ	C4-N4	4.74	1.45	1.33
1	A	129	CFZ	C2'-C3'	-4.74	1.46	1.52
1	A	439	CFZ	C4-N4	4.74	1.45	1.33
1	A	560	CFZ	C4-N4	4.74	1.45	1.33
1	A	75	CFZ	C4-N4	4.74	1.45	1.33
1	A	378	CFZ	C4-N4	4.74	1.45	1.33
1	A	663	CFZ	C4-N4	4.74	1.45	1.33
1	A	162	CFZ	C2'-C3'	-4.74	1.46	1.52
1	A	483	CFZ	C2'-C3'	-4.74	1.46	1.52
1	A	335	CFZ	C4-N4	4.73	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	625	CFZ	C4-N4	4.73	1.45	1.33
1	A	563	UFT	C2-N1	4.73	1.45	1.38
1	A	363	CFZ	C4-N4	4.73	1.45	1.33
1	A	694	CFZ	C4-N4	4.73	1.45	1.33
1	A	585	UFT	C2-N1	4.73	1.45	1.38
1	A	541	CFZ	C4-N4	4.73	1.45	1.33
1	A	88	UFT	C2-N1	4.73	1.45	1.38
1	A	644	UFT	C2-N1	4.73	1.45	1.38
1	A	616	UFT	C2-N1	4.73	1.45	1.38
1	A	204	CFZ	C4-N4	4.73	1.45	1.33
1	A	109	CFZ	C4-N4	4.73	1.45	1.33
1	A	685	CFZ	C4-N4	4.73	1.45	1.33
1	A	547	CFZ	C4-N4	4.73	1.45	1.33
1	A	146	CFZ	C4-N4	4.73	1.45	1.33
1	A	138	UFT	C2-N1	4.73	1.45	1.38
1	A	190	CFZ	C4-N4	4.73	1.45	1.33
1	A	275	CFZ	C4-N4	4.73	1.45	1.33
1	A	342	CFZ	C4-N4	4.73	1.45	1.33
1	A	624	UFT	C2-N1	4.73	1.45	1.38
1	A	484	CFZ	C2'-C3'	-4.73	1.46	1.52
1	A	101	CFZ	C4-N4	4.73	1.45	1.33
1	A	306	CFZ	C4-N4	4.73	1.45	1.33
1	A	135	CFZ	C4-N4	4.72	1.45	1.33
1	A	439	CFZ	C2'-C3'	-4.72	1.46	1.52
1	A	698	UFT	C2-N1	4.72	1.45	1.38
1	A	546	CFZ	C4-N4	4.72	1.45	1.33
1	A	359	CFZ	C4-N4	4.72	1.45	1.33
1	A	467	CFZ	C2'-C3'	-4.72	1.46	1.52
1	A	657	CFZ	C4-N4	4.72	1.45	1.33
1	A	690	CFZ	C4-N4	4.72	1.45	1.33
1	A	162	CFZ	C4-N4	4.72	1.45	1.33
1	A	433	CFZ	C4-N4	4.72	1.45	1.33
1	A	328	CFZ	C4-N4	4.72	1.45	1.33
1	A	343	CFZ	C4-N4	4.72	1.45	1.33
1	A	109	CFZ	C2'-C3'	-4.72	1.46	1.52
1	A	355	CFZ	C4-N4	4.72	1.45	1.33
1	A	600	CFZ	C4-N4	4.72	1.45	1.33
1	A	666	CFZ	C4-N4	4.72	1.45	1.33
1	A	604	CFZ	C4-N4	4.72	1.45	1.33
1	A	675	CFZ	C4-N4	4.72	1.45	1.33
1	A	217	CFZ	C2-N3	4.72	1.45	1.36
1	A	526	CFZ	C4-N4	4.72	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	UFT	C2-N1	4.72	1.45	1.38
1	A	635	CFZ	C2'-C3'	-4.72	1.46	1.52
1	A	269	CFZ	C4-N4	4.72	1.45	1.33
1	A	728	CFZ	C4-N4	4.71	1.45	1.33
1	A	32	UFT	C2-N1	4.71	1.45	1.38
1	A	143	UFT	C2-N1	4.71	1.45	1.38
1	A	157	CFZ	C4-N4	4.71	1.45	1.33
1	A	432	CFZ	C4-N4	4.71	1.45	1.33
1	A	178	CFZ	C2'-C3'	-4.71	1.46	1.52
1	A	397	UFT	C2-N1	4.71	1.45	1.38
1	A	515	CFZ	C4-N4	4.71	1.45	1.33
1	A	65	CFZ	C2'-C3'	-4.71	1.46	1.52
1	A	272	UFT	C2-N1	4.71	1.45	1.38
1	A	458	CFZ	C4-N4	4.71	1.45	1.33
1	A	706	CFZ	C4-N4	4.71	1.45	1.33
1	A	217	CFZ	C2'-C3'	-4.71	1.46	1.52
1	A	434	CFZ	C2'-C3'	-4.71	1.46	1.52
1	A	154	UFT	C2-N1	4.71	1.45	1.38
1	A	689	CFZ	C2'-C3'	-4.70	1.46	1.52
1	A	336	CFZ	C4-N4	4.70	1.45	1.33
1	A	34	CFZ	C4-N4	4.70	1.45	1.33
1	A	276	CFZ	C4-N4	4.70	1.45	1.33
1	A	506	CFZ	C4-N4	4.70	1.45	1.33
1	A	308	CFZ	C4-N4	4.70	1.45	1.33
1	A	437	CFZ	C4-N4	4.70	1.45	1.33
1	A	41	CFZ	C2'-C3'	-4.70	1.46	1.52
1	A	167	UFT	C2-N1	4.70	1.45	1.38
1	A	665	CFZ	C4-N4	4.70	1.45	1.33
1	A	696	CFZ	C4-N4	4.70	1.45	1.33
1	A	653	CFZ	C4-N4	4.70	1.45	1.33
1	A	242	UFT	C2-N1	4.70	1.45	1.38
1	A	383	UFT	C2-N1	4.70	1.45	1.38
1	A	630	CFZ	C4-N4	4.69	1.45	1.33
1	A	649	CFZ	C4-N4	4.69	1.45	1.33
1	A	379	CFZ	C2'-C3'	-4.69	1.46	1.52
1	A	629	CFZ	C4-N4	4.69	1.45	1.33
1	A	6	UFT	C2-N1	4.69	1.45	1.38
1	A	209	CFZ	C2'-C3'	-4.69	1.46	1.52
1	A	212	CFZ	C2'-C3'	-4.69	1.46	1.52
1	A	366	CFZ	C2'-C3'	-4.69	1.46	1.52
1	A	128	CFZ	C4-N4	4.69	1.45	1.33
1	A	458	CFZ	C2'-C3'	-4.69	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	CFZ	C4-N4	4.69	1.45	1.33
1	A	422	CFZ	C4-N4	4.69	1.45	1.33
1	A	273	CFZ	C4-N4	4.69	1.45	1.33
1	A	332	CFZ	C2'-C3'	-4.69	1.46	1.52
1	A	188	UFT	C6-N1	4.69	1.49	1.38
1	A	683	UFT	C2-N1	4.69	1.45	1.38
1	A	50	CFZ	C4-N4	4.69	1.45	1.33
1	A	219	CFZ	C4-N4	4.68	1.45	1.33
1	A	395	CFZ	C4-N4	4.68	1.45	1.33
1	A	10	CFZ	C2'-C3'	-4.68	1.46	1.52
1	A	314	CFZ	C4-N4	4.68	1.45	1.33
1	A	184	CFZ	C4-N4	4.68	1.45	1.33
1	A	217	CFZ	C4-N4	4.68	1.45	1.33
1	A	359	CFZ	C2'-C3'	-4.68	1.46	1.52
1	A	512	CFZ	C4-N4	4.68	1.45	1.33
1	A	577	CFZ	C4-N4	4.68	1.45	1.33
1	A	178	CFZ	C4-N4	4.68	1.45	1.33
1	A	12	CFZ	C2'-C3'	-4.68	1.46	1.52
1	A	501	UFT	C2-N1	4.68	1.45	1.38
1	A	489	CFZ	C4-N4	4.68	1.45	1.33
1	A	75	CFZ	C2'-C3'	-4.68	1.46	1.52
1	A	275	CFZ	C2'-C3'	-4.68	1.46	1.52
1	A	310	CFZ	C2'-C3'	-4.68	1.46	1.52
1	A	111	CFZ	C4-N4	4.68	1.45	1.33
1	A	256	CFZ	C4-N4	4.68	1.45	1.33
1	A	620	CFZ	C4-N4	4.68	1.45	1.33
1	A	417	UFT	C2-N1	4.68	1.45	1.38
1	A	532	UFT	C6-N1	4.68	1.49	1.38
1	A	181	UFT	C6-N1	4.67	1.49	1.38
1	A	522	CFZ	C4-N4	4.67	1.45	1.33
1	A	330	CFZ	C2'-C3'	-4.67	1.46	1.52
1	A	453	CFZ	C2'-C3'	-4.67	1.46	1.52
1	A	41	CFZ	C4-N4	4.67	1.45	1.33
1	A	192	UFT	C2-N1	4.67	1.45	1.38
1	A	332	CFZ	C4-N4	4.67	1.45	1.33
1	A	444	UFT	C6-N1	4.67	1.49	1.38
1	A	234	CFZ	C2-N3	4.67	1.45	1.36
1	A	434	CFZ	C4-N4	4.67	1.45	1.33
1	A	256	CFZ	C2'-C3'	-4.67	1.46	1.52
1	A	627	UFT	C6-N1	4.67	1.49	1.38
1	A	147	CFZ	C4-N4	4.67	1.45	1.33
1	A	518	CFZ	C4-N4	4.66	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	589	UFT	C2-N1	4.66	1.45	1.38
1	A	17	UFT	C6-N1	4.66	1.49	1.38
1	A	287	CFZ	C2'-C3'	-4.66	1.46	1.52
1	A	466	CFZ	C2'-C3'	-4.66	1.46	1.52
1	A	667	UFT	C2-N1	4.66	1.45	1.38
1	A	337	CFZ	C2'-C3'	-4.66	1.46	1.52
1	A	518	CFZ	C2'-C3'	-4.66	1.46	1.52
1	A	234	CFZ	C4-N4	4.66	1.45	1.33
1	A	97	UFT	C6-N1	4.66	1.49	1.38
1	A	79	UFT	C2-N1	4.66	1.45	1.38
1	A	512	CFZ	C2'-C3'	-4.65	1.46	1.52
1	A	560	CFZ	C2'-C3'	-4.65	1.46	1.52
1	A	345	UFT	C2-N1	4.65	1.45	1.38
1	A	298	UFT	C6-N1	4.65	1.49	1.38
1	A	582	UFT	C6-N1	4.65	1.49	1.38
1	A	137	CFZ	C2'-C3'	-4.65	1.46	1.52
1	A	46	UFT	C6-N1	4.65	1.49	1.38
1	A	355	CFZ	C2'-C3'	-4.65	1.46	1.52
1	A	531	CFZ	C4-N4	4.65	1.45	1.33
1	A	405	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	291	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	625	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	382	CFZ	C4-N4	4.64	1.45	1.33
1	A	221	UFT	C6-N1	4.64	1.49	1.38
1	A	665	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	80	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	670	UFT	C2-N1	4.64	1.45	1.38
1	A	351	UFT	C2-N1	4.64	1.45	1.38
1	A	686	UFT	C6-N1	4.64	1.49	1.38
1	A	11	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	131	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	244	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	336	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	142	UFT	C2-N1	4.64	1.45	1.38
1	A	649	CFZ	C2'-C3'	-4.64	1.46	1.52
1	A	475	UFT	C6-N1	4.63	1.49	1.38
1	A	463	CFZ	C2-N3	4.63	1.45	1.36
1	A	196	UFT	C2-N1	4.63	1.45	1.38
1	A	322	UFT	C2-N1	4.63	1.45	1.38
1	A	130	CFZ	C4-N4	4.63	1.45	1.33
1	A	437	CFZ	C2'-C3'	-4.63	1.46	1.52
1	A	637	CFZ	C4-N4	4.63	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	CFZ	C2'-C3'	-4.63	1.46	1.52
1	A	432	CFZ	C2'-C3'	-4.63	1.46	1.52
1	A	148	UFT	C6-N1	4.63	1.49	1.38
1	A	386	CFZ	C2'-C3'	-4.63	1.46	1.52
1	A	557	CFZ	C4-N4	4.63	1.45	1.33
1	A	480	UFT	C2-N1	4.62	1.45	1.38
1	A	497	UFT	C2'-C3'	-4.62	1.46	1.52
1	A	429	UFT	C6-N1	4.62	1.49	1.38
1	A	655	UFT	C6-N1	4.62	1.49	1.38
1	A	709	CFZ	C2-N3	4.62	1.45	1.36
1	A	388	UFT	C6-N1	4.62	1.49	1.38
1	A	15	CFZ	C2'-C3'	-4.62	1.46	1.52
1	A	549	UFT	C6-N1	4.62	1.49	1.38
1	A	557	CFZ	C2'-C3'	-4.62	1.46	1.52
1	A	208	CFZ	C2'-C3'	-4.61	1.46	1.52
1	A	240	UFT	C6-N1	4.61	1.49	1.38
1	A	344	CFZ	C2'-C3'	-4.61	1.46	1.52
1	A	416	CFZ	C2-N3	4.61	1.45	1.36
1	A	350	UFT	C6-N1	4.61	1.49	1.38
1	A	416	CFZ	C4-N4	4.61	1.45	1.33
1	A	527	CFZ	C2'-C3'	-4.61	1.46	1.52
1	A	382	CFZ	C2'-C3'	-4.61	1.46	1.52
1	A	417	UFT	C6-N1	4.61	1.49	1.38
1	A	607	UFT	C6-N1	4.61	1.49	1.38
1	A	555	UFT	C6-N1	4.60	1.49	1.38
1	A	642	UFT	C6-N1	4.60	1.49	1.38
1	A	598	CFZ	C2'-C3'	-4.60	1.46	1.52
1	A	48	UFT	C6-N1	4.60	1.49	1.38
1	A	197	UFT	C6-N1	4.60	1.49	1.38
1	A	727	UFT	C6-N1	4.60	1.49	1.38
1	A	363	CFZ	C2'-C3'	-4.60	1.46	1.52
1	A	238	UFT	C6-N1	4.60	1.49	1.38
1	A	87	CFZ	C2'-C3'	-4.60	1.46	1.52
1	A	343	CFZ	C2'-C3'	-4.60	1.46	1.52
1	A	397	UFT	C6-N1	4.60	1.49	1.38
1	A	89	UFT	C2-N1	4.60	1.45	1.38
1	A	115	UFT	C2-N1	4.60	1.45	1.38
1	A	39	UFT	C6-N1	4.60	1.49	1.38
1	A	563	UFT	C6-N1	4.60	1.49	1.38
1	A	335	CFZ	C2'-C3'	-4.60	1.46	1.52
1	A	521	UFT	C2-N1	4.60	1.45	1.38
1	A	170	UFT	C6-N1	4.60	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	662	UFT	C6-N1	4.59	1.49	1.38
1	A	510	UFT	C2-N1	4.59	1.45	1.38
1	A	151	UFT	C6-N1	4.59	1.49	1.38
1	A	589	UFT	C6-N1	4.59	1.49	1.38
1	A	177	UFT	C6-N1	4.59	1.49	1.38
1	A	497	UFT	C6-N1	4.59	1.49	1.38
1	A	562	UFT	C6-N1	4.59	1.49	1.38
1	A	83	CFZ	C2'-C3'	-4.59	1.46	1.52
1	A	107	UFT	C6-N1	4.59	1.49	1.38
1	A	489	CFZ	C2'-C3'	-4.59	1.46	1.52
1	A	456	CFZ	C2'-C3'	-4.59	1.46	1.52
1	A	219	CFZ	C2-N3	4.59	1.45	1.36
1	A	598	CFZ	C2-N3	4.59	1.45	1.36
1	A	6	UFT	C6-N1	4.59	1.49	1.38
1	A	507	UFT	C6-N1	4.59	1.49	1.38
1	A	693	UFT	C6-N1	4.59	1.49	1.38
1	A	709	CFZ	C4-N4	4.59	1.45	1.33
1	A	468	UFT	C6-N1	4.59	1.49	1.38
1	A	161	CFZ	C2'-C3'	-4.59	1.46	1.52
1	A	709	CFZ	C2'-C3'	-4.59	1.46	1.52
1	A	339	UFT	C6-N1	4.59	1.49	1.38
1	A	319	UFT	C6-N1	4.58	1.49	1.38
1	A	215	UFT	C6-N1	4.58	1.49	1.38
1	A	616	UFT	C6-N1	4.58	1.49	1.38
1	A	154	UFT	C6-N1	4.58	1.49	1.38
1	A	643	UFT	C6-N1	4.58	1.49	1.38
1	A	444	UFT	C2-N1	4.58	1.45	1.38
1	A	501	UFT	C6-N1	4.58	1.49	1.38
1	A	510	UFT	C6-N1	4.58	1.49	1.38
1	A	617	UFT	C6-N1	4.58	1.49	1.38
1	A	32	UFT	C6-N1	4.58	1.49	1.38
1	A	103	CFZ	C4-N4	4.58	1.45	1.33
1	A	476	UFT	C6-N1	4.58	1.49	1.38
1	A	190	CFZ	C2'-C3'	-4.57	1.46	1.52
1	A	103	CFZ	C2'-C3'	-4.57	1.46	1.52
1	A	641	CFZ	C2'-C3'	-4.57	1.46	1.52
1	A	575	UFT	C6-N1	4.57	1.49	1.38
1	A	653	CFZ	C2'-C3'	-4.57	1.46	1.52
1	A	23	UFT	C6-N1	4.57	1.49	1.38
1	A	33	UFT	C6-N1	4.57	1.49	1.38
1	A	383	UFT	C6-N1	4.57	1.49	1.38
1	A	573	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	19	UFT	C6-N1	4.57	1.49	1.38
1	A	451	UFT	C6-N1	4.57	1.49	1.38
1	A	61	UFT	C6-N1	4.57	1.49	1.38
1	A	419	UFT	C6-N1	4.57	1.49	1.38
1	A	173	CFZ	C2'-C3'	-4.57	1.46	1.52
1	A	437	CFZ	C2-N3	4.57	1.45	1.36
1	A	307	UFT	C6-N1	4.57	1.49	1.38
1	A	679	UFT	C6-N1	4.57	1.49	1.38
1	A	367	UFT	C6-N1	4.57	1.49	1.38
1	A	480	UFT	C6-N1	4.57	1.49	1.38
1	A	671	UFT	C6-N1	4.57	1.49	1.38
1	A	79	UFT	C6-N1	4.57	1.49	1.38
1	A	395	CFZ	C2'-C3'	-4.56	1.46	1.52
1	A	476	UFT	C2-N1	4.56	1.45	1.38
1	A	267	UFT	C6-N1	4.56	1.49	1.38
1	A	121	CFZ	C2'-C3'	-4.56	1.46	1.52
1	A	116	UFT	C6-N1	4.56	1.49	1.38
1	A	272	UFT	C6-N1	4.56	1.49	1.38
1	A	600	CFZ	C2'-C3'	-4.56	1.46	1.52
1	A	115	UFT	C6-N1	4.56	1.49	1.38
1	A	434	CFZ	C2-N3	4.56	1.45	1.36
1	A	621	CFZ	C2'-C3'	-4.56	1.46	1.52
1	A	89	UFT	C6-N1	4.56	1.49	1.38
1	A	582	UFT	C2-N1	4.56	1.45	1.38
1	A	484	CFZ	C2-N3	4.56	1.45	1.36
1	A	522	CFZ	C2'-C3'	-4.56	1.46	1.52
1	A	717	CFZ	C4-N4	4.56	1.44	1.33
1	A	590	UFT	C6-N1	4.55	1.48	1.38
1	A	416	CFZ	C2'-C3'	-4.55	1.46	1.52
1	A	274	UFT	C6-N1	4.55	1.48	1.38
1	A	283	UFT	C6-N1	4.55	1.48	1.38
1	A	697	UFT	C6-N1	4.55	1.48	1.38
1	A	311	UFT	C6-N1	4.55	1.48	1.38
1	A	127	UFT	C6-N1	4.55	1.48	1.38
1	A	167	UFT	C6-N1	4.55	1.48	1.38
1	A	607	UFT	C2'-C3'	-4.55	1.46	1.52
1	A	515	CFZ	C2-N3	4.55	1.45	1.36
1	A	71	UFT	C6-N1	4.55	1.48	1.38
1	A	233	CFZ	C2'-C3'	-4.55	1.46	1.52
1	A	169	UFT	C6-N1	4.55	1.48	1.38
1	A	585	UFT	C6-N1	4.55	1.48	1.38
1	A	130	CFZ	C2'-C3'	-4.55	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	UFT	C2-N1	4.55	1.45	1.38
1	A	62	UFT	C6-N1	4.55	1.48	1.38
1	A	370	UFT	C6-N1	4.55	1.48	1.38
1	A	242	UFT	C6-N1	4.55	1.48	1.38
1	A	45	CFZ	C2'-C3'	-4.55	1.46	1.52
1	A	705	UFT	C2-N1	4.55	1.45	1.38
1	A	644	UFT	C6-N1	4.54	1.48	1.38
1	A	263	UFT	C6-N1	4.54	1.48	1.38
1	A	724	UFT	C6-N1	4.54	1.48	1.38
1	A	562	UFT	C2-N1	4.54	1.45	1.38
1	A	670	UFT	C6-N1	4.54	1.48	1.38
1	A	192	UFT	C6-N1	4.54	1.48	1.38
1	A	369	CFZ	C2'-C3'	-4.54	1.46	1.52
1	A	138	UFT	C6-N1	4.54	1.48	1.38
1	A	254	UFT	C6-N1	4.54	1.48	1.38
1	A	719	UFT	C6-N1	4.54	1.48	1.38
1	A	88	UFT	C6-N1	4.54	1.48	1.38
1	A	345	UFT	C6-N1	4.54	1.48	1.38
1	A	685	CFZ	C2'-C3'	-4.54	1.46	1.52
1	A	44	UFT	C6-N1	4.54	1.48	1.38
1	A	382	CFZ	C2-N3	4.54	1.45	1.36
1	A	438	CFZ	C2'-C3'	-4.54	1.46	1.52
1	A	588	UFT	C6-N1	4.53	1.48	1.38
1	A	665	CFZ	C2-N3	4.53	1.45	1.36
1	A	431	UFT	C6-N1	4.53	1.48	1.38
1	A	271	CFZ	C2'-C3'	-4.53	1.46	1.52
1	A	409	UFT	C6-N1	4.53	1.48	1.38
1	A	94	UFT	C6-N1	4.53	1.48	1.38
1	A	432	CFZ	C2-N3	4.53	1.45	1.36
1	A	526	CFZ	C2'-C3'	-4.53	1.46	1.52
1	A	196	UFT	C6-N1	4.52	1.48	1.38
1	A	26	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	204	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	123	UFT	C6-N1	4.52	1.48	1.38
1	A	111	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	42	UFT	C6-N1	4.52	1.48	1.38
1	A	271	CFZ	C2-N3	4.52	1.45	1.36
1	A	512	CFZ	C2-N3	4.52	1.45	1.36
1	A	502	CFZ	C2'-C3'	-4.52	1.46	1.52
1	A	143	UFT	C6-N1	4.51	1.48	1.38
1	A	637	CFZ	C2'-C3'	-4.51	1.46	1.52
1	A	11	CFZ	C2-N3	4.51	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	523	UFT	C6-N1	4.51	1.48	1.38
1	A	695	CFZ	C2'-C3'	-4.51	1.46	1.52
1	A	173	CFZ	C2-N3	4.51	1.45	1.36
1	A	329	UFT	C6-N1	4.51	1.48	1.38
1	A	698	UFT	C6-N1	4.51	1.48	1.38
1	A	557	CFZ	C2-N3	4.51	1.45	1.36
1	A	303	UFT	C6-N1	4.51	1.48	1.38
1	A	556	UFT	C6-N1	4.51	1.48	1.38
1	A	184	CFZ	C2'-C3'	-4.51	1.46	1.52
1	A	624	UFT	C6-N1	4.51	1.48	1.38
1	A	705	UFT	C6-N1	4.51	1.48	1.38
1	A	208	CFZ	C2-N3	4.50	1.45	1.36
1	A	657	CFZ	C2'-C3'	-4.50	1.46	1.52
1	A	142	UFT	C6-N1	4.50	1.48	1.38
1	A	50	CFZ	C2'-C3'	-4.50	1.46	1.52
1	A	360	UFT	C6-N1	4.50	1.48	1.38
1	A	81	CFZ	C2'-C3'	-4.50	1.46	1.52
1	A	485	UFT	C6-N1	4.50	1.48	1.38
1	A	504	UFT	C6-N1	4.50	1.48	1.38
1	A	499	CFZ	C2'-C3'	-4.50	1.46	1.52
1	A	390	UFT	C6-N1	4.50	1.48	1.38
1	A	181	UFT	C2-N1	4.50	1.45	1.38
1	A	713	CFZ	C2-N3	4.50	1.45	1.36
1	A	130	CFZ	C2-N3	4.50	1.45	1.36
1	A	609	CFZ	C2'-C3'	-4.50	1.46	1.52
1	A	120	UFT	C6-N1	4.49	1.48	1.38
1	A	421	UFT	C6-N1	4.49	1.48	1.38
1	A	607	UFT	C2-N1	4.49	1.45	1.38
1	A	522	CFZ	C2-N3	4.49	1.45	1.36
1	A	374	UFT	C6-N1	4.49	1.48	1.38
1	A	58	UFT	C6-N1	4.49	1.48	1.38
1	A	230	UFT	C6-N1	4.49	1.48	1.38
1	A	604	CFZ	C2'-C3'	-4.49	1.46	1.52
1	A	559	UFT	C6-N1	4.48	1.48	1.38
1	A	173	CFZ	C4-N4	4.48	1.44	1.33
1	A	493	CFZ	C2'-C3'	-4.48	1.46	1.52
1	A	632	CFZ	C2'-C3'	-4.48	1.46	1.52
1	A	288	UFT	C6-N1	4.48	1.48	1.38
1	A	464	UFT	C6-N1	4.48	1.48	1.38
1	A	314	CFZ	C2'-C3'	-4.48	1.46	1.52
1	A	699	CFZ	C2'-C3'	-4.48	1.46	1.52
1	A	609	CFZ	C2-N3	4.48	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	UFT	C6-N1	4.48	1.48	1.38
1	A	518	CFZ	C2-N3	4.48	1.45	1.36
1	A	433	CFZ	C2'-C3'	-4.48	1.46	1.52
1	A	542	UFT	C6-N1	4.48	1.48	1.38
1	A	157	CFZ	C2'-C3'	-4.48	1.46	1.52
1	A	663	CFZ	C2'-C3'	-4.48	1.46	1.52
1	A	273	CFZ	C2-N3	4.47	1.45	1.36
1	A	114	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	351	UFT	C6-N1	4.47	1.48	1.38
1	A	236	UFT	C6-N1	4.47	1.48	1.38
1	A	683	UFT	C6-N1	4.47	1.48	1.38
1	A	597	UFT	C6-N1	4.47	1.48	1.38
1	A	182	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	601	UFT	C6-N1	4.47	1.48	1.38
1	A	175	UFT	C6-N1	4.47	1.48	1.38
1	A	713	CFZ	C2'-C3'	-4.47	1.46	1.52
1	A	51	UFT	C6-N1	4.47	1.48	1.38
1	A	550	UFT	C6-N1	4.46	1.48	1.38
1	A	391	CFZ	C2'-C3'	-4.46	1.46	1.52
1	A	392	CFZ	C2'-C3'	-4.46	1.46	1.52
1	A	602	CFZ	C2'-C3'	-4.46	1.46	1.52
1	A	93	UFT	C6-N1	4.46	1.48	1.38
1	A	153	CFZ	C2'-C3'	-4.46	1.46	1.52
1	A	342	CFZ	C2-N3	4.46	1.45	1.36
1	A	439	CFZ	C2-N3	4.46	1.45	1.36
1	A	111	CFZ	C2-N3	4.46	1.45	1.36
1	A	194	UFT	C6-N1	4.46	1.48	1.38
1	A	612	UFT	C6-N1	4.46	1.48	1.38
1	A	561	CFZ	C2'-C3'	-4.46	1.46	1.52
1	A	73	CFZ	C2-N3	4.45	1.45	1.36
1	A	661	CFZ	C2'-C3'	-4.45	1.46	1.52
1	A	58	UFT	C2-N1	4.45	1.45	1.38
1	A	340	UFT	C6-N1	4.45	1.48	1.38
1	A	56	UFT	C6-N1	4.45	1.48	1.38
1	A	221	UFT	C2'-C3'	-4.45	1.46	1.52
1	A	595	UFT	C6-N1	4.45	1.48	1.38
1	A	717	CFZ	C2-N3	4.44	1.45	1.36
1	A	558	UFT	C6-N1	4.44	1.48	1.38
1	A	75	CFZ	C2-N3	4.44	1.45	1.36
1	A	429	UFT	C2'-C3'	-4.44	1.46	1.52
1	A	12	CFZ	C2-N3	4.44	1.45	1.36
1	A	582	UFT	C2'-C3'	-4.44	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	CFZ	C2-N3	4.44	1.45	1.36
1	A	666	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	630	CFZ	C2'-C3'	-4.44	1.46	1.52
1	A	638	UFT	C6-N1	4.43	1.48	1.38
1	A	165	CFZ	C2-N3	4.43	1.45	1.36
1	A	147	CFZ	C2'-C3'	-4.43	1.46	1.52
1	A	302	CFZ	C2'-C3'	-4.43	1.46	1.52
1	A	724	UFT	C2-N1	4.43	1.45	1.38
1	A	460	CFZ	C2'-C3'	-4.43	1.46	1.52
1	A	101	CFZ	C2-N3	4.43	1.45	1.36
1	A	273	CFZ	C2'-C3'	-4.42	1.46	1.52
1	A	521	UFT	C6-N1	4.42	1.48	1.38
1	A	407	CFZ	C2'-C3'	-4.42	1.46	1.52
1	A	359	CFZ	C2-N3	4.42	1.45	1.36
1	A	63	CFZ	C2'-C3'	-4.42	1.46	1.52
1	A	603	CFZ	C2'-C3'	-4.42	1.46	1.52
1	A	666	CFZ	C2-N3	4.42	1.45	1.36
1	A	212	CFZ	C2-N3	4.42	1.45	1.36
1	A	471	UFT	C6-N1	4.42	1.48	1.38
1	A	532	UFT	C2-N1	4.41	1.45	1.38
1	A	637	CFZ	C2-N3	4.41	1.45	1.36
1	A	658	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	108	CFZ	C2-N3	4.41	1.45	1.36
1	A	190	CFZ	C2-N3	4.41	1.45	1.36
1	A	577	CFZ	C2-N3	4.41	1.45	1.36
1	A	690	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	206	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	276	CFZ	C2-N3	4.41	1.45	1.36
1	A	685	CFZ	C2-N3	4.41	1.45	1.36
1	A	156	CFZ	C2-N3	4.41	1.45	1.36
1	A	672	CFZ	C2'-C3'	-4.41	1.46	1.52
1	A	95	UFT	C6-N1	4.40	1.48	1.38
1	A	526	CFZ	C2-N3	4.40	1.45	1.36
1	A	362	CFZ	C2'-C3'	-4.40	1.46	1.52
1	A	328	CFZ	C2-N3	4.40	1.45	1.36
1	A	499	CFZ	C2-N3	4.40	1.45	1.36
1	A	165	CFZ	C2'-C3'	-4.40	1.46	1.52
1	A	687	UFT	C6-N1	4.40	1.48	1.38
1	A	577	CFZ	C2'-C3'	-4.40	1.46	1.52
1	A	379	CFZ	C2-N3	4.40	1.45	1.36
1	A	322	UFT	C6-N1	4.40	1.48	1.38
1	A	649	CFZ	C2-N3	4.40	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	UFT	C6-N1	4.40	1.48	1.38
1	A	361	UFT	C6-N1	4.39	1.48	1.38
1	A	154	UFT	C5-C4	4.39	1.53	1.43
1	A	515	CFZ	C2'-C3'	-4.39	1.46	1.52
1	A	588	UFT	C2-N1	4.39	1.45	1.38
1	A	306	CFZ	C2-N3	4.39	1.45	1.36
1	A	667	UFT	C6-N1	4.39	1.48	1.38
1	A	720	CFZ	C2-N3	4.39	1.45	1.36
1	A	631	CFZ	C2-N3	4.39	1.45	1.36
1	A	706	CFZ	C2-N3	4.38	1.45	1.36
1	A	458	CFZ	C2-N3	4.38	1.45	1.36
1	A	473	CFZ	C2-N3	4.38	1.45	1.36
1	A	645	CFZ	C2'-C3'	-4.38	1.46	1.52
1	A	137	CFZ	C2-N3	4.38	1.45	1.36
1	A	291	CFZ	C2-N3	4.38	1.45	1.36
1	A	28	CFZ	C2-N3	4.38	1.45	1.36
1	A	129	CFZ	C2-N3	4.38	1.45	1.36
1	A	467	CFZ	C2-N3	4.38	1.45	1.36
1	A	181	UFT	C5-C4	4.38	1.53	1.43
1	A	41	CFZ	C2-N3	4.38	1.45	1.36
1	A	613	CFZ	C2'-C3'	-4.38	1.46	1.52
1	A	456	CFZ	C2-N3	4.38	1.45	1.36
1	A	564	CFZ	C2'-C3'	-4.37	1.46	1.52
1	A	355	CFZ	C2-N3	4.37	1.45	1.36
1	A	378	CFZ	C2-N3	4.37	1.45	1.36
1	A	656	CFZ	C2'-C3'	-4.37	1.46	1.52
1	A	690	CFZ	C2-N3	4.37	1.45	1.36
1	A	561	CFZ	C2-N3	4.37	1.45	1.36
1	A	72	CFZ	C2'-C3'	-4.37	1.46	1.52
1	A	10	CFZ	C2-N3	4.37	1.45	1.36
1	A	34	CFZ	C2-N3	4.37	1.45	1.36
1	A	442	CFZ	C2-N3	4.37	1.45	1.36
1	A	83	CFZ	C2-N3	4.36	1.45	1.36
1	A	391	CFZ	C2-N3	4.36	1.45	1.36
1	A	426	CFZ	C2'-C3'	-4.36	1.46	1.52
1	A	663	CFZ	C2-N3	4.36	1.45	1.36
1	A	233	CFZ	C2-N3	4.36	1.45	1.36
1	A	438	CFZ	C2-N3	4.36	1.45	1.36
1	A	276	CFZ	C2'-C3'	-4.36	1.46	1.52
1	A	582	UFT	C5-C4	4.36	1.53	1.43
1	A	716	UFT	C5-C4	4.36	1.53	1.43
1	A	210	UFT	C6-N1	4.36	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	CFZ	C2'-C3'	-4.36	1.46	1.52
1	A	675	CFZ	C2'-C3'	-4.36	1.46	1.52
1	A	575	UFT	C2'-C3'	-4.36	1.46	1.52
1	A	204	CFZ	C2-N3	4.35	1.45	1.36
1	A	314	CFZ	C2-N3	4.35	1.45	1.36
1	A	686	UFT	C5-C4	4.35	1.53	1.43
1	A	45	CFZ	C2-N3	4.35	1.45	1.36
1	A	384	CFZ	C2-N3	4.35	1.45	1.36
1	A	466	CFZ	C2-N3	4.35	1.45	1.36
1	A	532	UFT	C5-C4	4.35	1.53	1.43
1	A	117	CFZ	C2'-C3'	-4.35	1.46	1.52
1	A	193	UFT	C6-N1	4.35	1.48	1.38
1	A	650	UFT	C6-N1	4.35	1.48	1.38
1	A	144	CFZ	C2'-C3'	-4.35	1.47	1.52
1	A	161	CFZ	C2-N3	4.35	1.45	1.36
1	A	114	CFZ	C2-N3	4.35	1.45	1.36
1	A	107	UFT	C2'-C3'	-4.34	1.47	1.52
1	A	340	UFT	C2'-C3'	-4.34	1.47	1.52
1	A	103	CFZ	C2-N3	4.34	1.45	1.36
1	A	162	CFZ	C2-N3	4.34	1.45	1.36
1	A	256	CFZ	C2-N3	4.34	1.45	1.36
1	A	206	CFZ	C2-N3	4.34	1.45	1.36
1	A	178	CFZ	C2-N3	4.34	1.45	1.36
1	A	500	CFZ	C2-N3	4.34	1.45	1.36
1	A	547	CFZ	C2-N3	4.34	1.45	1.36
1	A	151	UFT	C5-C4	4.34	1.53	1.43
1	A	335	CFZ	C2-N3	4.34	1.45	1.36
1	A	497	UFT	C5-C4	4.34	1.53	1.43
1	A	311	UFT	C5-C4	4.34	1.53	1.43
1	A	444	UFT	C5-C4	4.34	1.53	1.43
1	A	661	CFZ	C2-N3	4.34	1.44	1.36
1	A	370	UFT	C5-C4	4.34	1.53	1.43
1	A	336	CFZ	C2-N3	4.33	1.44	1.36
1	A	337	CFZ	C2-N3	4.33	1.44	1.36
1	A	343	CFZ	C2-N3	4.33	1.44	1.36
1	A	674	CFZ	C2'-C3'	-4.33	1.47	1.52
1	A	66	UFT	C6-N1	4.33	1.48	1.38
1	A	104	CFZ	C2-N3	4.33	1.44	1.36
1	A	422	CFZ	C2-N3	4.33	1.44	1.36
1	A	311	UFT	C2'-C3'	-4.33	1.47	1.52
1	A	487	CFZ	C2-N3	4.33	1.44	1.36
1	A	635	CFZ	C2-N3	4.33	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	607	UFT	C5-C4	4.33	1.53	1.43
1	A	155	CFZ	C2'-C3'	-4.33	1.47	1.52
1	A	489	CFZ	C2-N3	4.33	1.44	1.36
1	A	695	CFZ	C2-N3	4.33	1.44	1.36
1	A	728	CFZ	C2-N3	4.33	1.44	1.36
1	A	621	CFZ	C2-N3	4.33	1.44	1.36
1	A	298	UFT	C5-C4	4.33	1.53	1.43
1	A	57	CFZ	C2-N3	4.32	1.44	1.36
1	A	501	UFT	C5-C4	4.32	1.53	1.43
1	A	131	CFZ	C2-N3	4.32	1.44	1.36
1	A	332	CFZ	C2-N3	4.32	1.44	1.36
1	A	442	CFZ	C2'-C3'	-4.32	1.47	1.52
1	A	109	CFZ	C2-N3	4.32	1.44	1.36
1	A	127	UFT	C5-C4	4.32	1.53	1.43
1	A	536	CFZ	C2-N3	4.32	1.44	1.36
1	A	696	CFZ	C2-N3	4.31	1.44	1.36
1	A	632	CFZ	C2-N3	4.31	1.44	1.36
1	A	310	CFZ	C2-N3	4.31	1.44	1.36
1	A	213	UFT	C6-N1	4.31	1.48	1.38
1	A	88	UFT	C5-C4	4.31	1.53	1.43
1	A	527	CFZ	C2-N3	4.31	1.44	1.36
1	A	346	CFZ	C2-N3	4.31	1.44	1.36
1	A	32	UFT	C5-C4	4.31	1.53	1.43
1	A	620	CFZ	C2'-C3'	-4.30	1.47	1.52
1	A	184	CFZ	C2-N3	4.30	1.44	1.36
1	A	298	UFT	C2'-C3'	-4.30	1.47	1.52
1	A	613	CFZ	C2-N3	4.30	1.44	1.36
1	A	727	UFT	C5-C4	4.30	1.53	1.43
1	A	417	UFT	C5-C4	4.30	1.53	1.43
1	A	662	UFT	C5-C4	4.30	1.53	1.43
1	A	397	UFT	C5-C4	4.30	1.53	1.43
1	A	371	UFT	C6-N1	4.30	1.48	1.38
1	A	362	CFZ	C2-N3	4.30	1.44	1.36
1	A	171	CFZ	C2'-C3'	-4.30	1.47	1.52
1	A	147	CFZ	C2-N3	4.30	1.44	1.36
1	A	195	CFZ	C2-N3	4.29	1.44	1.36
1	A	115	UFT	C5-C4	4.29	1.53	1.43
1	A	589	UFT	C5-C4	4.29	1.53	1.43
1	A	240	UFT	C5-C4	4.29	1.53	1.43
1	A	209	CFZ	C2-N3	4.29	1.44	1.36
1	A	344	CFZ	C2-N3	4.29	1.44	1.36
1	A	655	UFT	C5-C4	4.29	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	UFT	C2'-C3'	-4.29	1.47	1.52
1	A	7	CFZ	C2-N3	4.29	1.44	1.36
1	A	269	CFZ	C2'-C3'	-4.29	1.47	1.52
1	A	588	UFT	C5-C4	4.29	1.53	1.43
1	A	689	CFZ	C2-N3	4.29	1.44	1.36
1	A	573	UFT	C2'-C3'	-4.29	1.47	1.52
1	A	604	CFZ	C2-N3	4.29	1.44	1.36
1	A	107	UFT	C5-C4	4.29	1.53	1.43
1	A	630	CFZ	C2-N3	4.28	1.44	1.36
1	A	433	CFZ	C2-N3	4.28	1.44	1.36
1	A	476	UFT	C5-C4	4.28	1.53	1.43
1	A	616	UFT	C5-C4	4.28	1.53	1.43
1	A	693	UFT	C2'-C3'	-4.28	1.47	1.52
1	A	653	CFZ	C2-N3	4.28	1.44	1.36
1	A	215	UFT	C5-C4	4.28	1.53	1.43
1	A	597	UFT	C5-C4	4.28	1.53	1.43
1	A	308	CFZ	C2-N3	4.28	1.44	1.36
1	A	238	UFT	C5-C4	4.28	1.53	1.43
1	A	319	UFT	C5-C4	4.28	1.53	1.43
1	A	80	CFZ	C2-N3	4.28	1.44	1.36
1	A	135	CFZ	C2-N3	4.28	1.44	1.36
1	A	407	CFZ	C2-N3	4.28	1.44	1.36
1	A	195	CFZ	C2'-C3'	-4.28	1.47	1.52
1	A	697	UFT	C5-C4	4.28	1.53	1.43
1	A	453	CFZ	C2-N3	4.28	1.44	1.36
1	A	698	UFT	C5-C4	4.28	1.53	1.43
1	A	50	CFZ	C2-N3	4.28	1.44	1.36
1	A	76	CFZ	C2-N3	4.27	1.44	1.36
1	A	48	UFT	C2'-C3'	-4.27	1.47	1.52
1	A	562	UFT	C5-C4	4.27	1.53	1.43
1	A	490	CFZ	C2-N3	4.27	1.44	1.36
1	A	675	CFZ	C2-N3	4.27	1.44	1.36
1	A	142	UFT	C5-C4	4.27	1.53	1.43
1	A	153	CFZ	C2-N3	4.27	1.44	1.36
1	A	62	UFT	C5-C4	4.27	1.53	1.43
1	A	269	CFZ	C2-N3	4.27	1.44	1.36
1	A	541	CFZ	C2-N3	4.27	1.44	1.36
1	A	451	UFT	C5-C4	4.27	1.53	1.43
1	A	345	UFT	C5-C4	4.27	1.53	1.43
1	A	720	CFZ	C2'-C3'	-4.27	1.47	1.52
1	A	79	UFT	C5-C4	4.27	1.53	1.43
1	A	367	UFT	C5-C4	4.26	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	UFT	C5-C4	4.26	1.53	1.43
1	A	620	CFZ	C2-N3	4.26	1.44	1.36
1	A	563	UFT	C5-C4	4.26	1.53	1.43
1	A	128	CFZ	C2-N3	4.26	1.44	1.36
1	A	510	UFT	C5-C4	4.26	1.53	1.43
1	A	51	UFT	C5-C4	4.26	1.52	1.43
1	A	705	UFT	C5-C4	4.26	1.52	1.43
1	A	329	UFT	C5-C4	4.26	1.52	1.43
1	A	670	UFT	C5-C4	4.26	1.52	1.43
1	A	288	UFT	C5-C4	4.26	1.52	1.43
1	A	480	UFT	C5-C4	4.26	1.52	1.43
1	A	6	UFT	C5-C4	4.26	1.52	1.43
1	A	578	CFZ	C2-N3	4.26	1.44	1.36
1	A	507	UFT	C5-C4	4.25	1.52	1.43
1	A	287	CFZ	C2-N3	4.25	1.44	1.36
1	A	555	UFT	C2'-C3'	-4.25	1.47	1.52
1	A	429	UFT	C5-C4	4.25	1.52	1.43
1	A	693	UFT	C5-C4	4.25	1.52	1.43
1	A	244	CFZ	C2-N3	4.25	1.44	1.36
1	A	600	CFZ	C2-N3	4.25	1.44	1.36
1	A	618	CFZ	C2'-C3'	-4.25	1.47	1.52
1	A	558	UFT	C2'-C3'	-4.25	1.47	1.52
1	A	452	CFZ	C2-N3	4.25	1.44	1.36
1	A	143	UFT	C5-C4	4.25	1.52	1.43
1	A	679	UFT	C5-C4	4.25	1.52	1.43
1	A	521	UFT	C2'-C3'	-4.25	1.47	1.52
1	A	644	UFT	C5-C4	4.25	1.52	1.43
1	A	451	UFT	C2'-C3'	-4.25	1.47	1.52
1	A	196	UFT	C5-C4	4.25	1.52	1.43
1	A	575	UFT	C5-C4	4.25	1.52	1.43
1	A	366	CFZ	C2-N3	4.25	1.44	1.36
1	A	123	UFT	C5-C4	4.25	1.52	1.43
1	A	330	CFZ	C2-N3	4.25	1.44	1.36
1	A	138	UFT	C5-C4	4.24	1.52	1.43
1	A	219	CFZ	C2'-C3'	-4.24	1.47	1.52
1	A	302	CFZ	C2-N3	4.24	1.44	1.36
1	A	392	CFZ	C2-N3	4.24	1.44	1.36
1	A	417	UFT	C2'-C3'	-4.24	1.47	1.52
1	A	33	UFT	C5-C4	4.24	1.52	1.43
1	A	617	UFT	C5-C4	4.24	1.52	1.43
1	A	395	CFZ	C2-N3	4.24	1.44	1.36
1	A	267	UFT	C5-C4	4.24	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	UFT	C5-C4	4.24	1.52	1.43
1	A	277	UFT	C5-C4	4.24	1.52	1.43
1	A	421	UFT	C5-C4	4.24	1.52	1.43
1	A	719	UFT	C5-C4	4.24	1.52	1.43
1	A	531	CFZ	C2-N3	4.24	1.44	1.36
1	A	272	UFT	C5-C4	4.24	1.52	1.43
1	A	350	UFT	C5-C4	4.24	1.52	1.43
1	A	58	UFT	C5-C4	4.24	1.52	1.43
1	A	388	UFT	C5-C4	4.24	1.52	1.43
1	A	464	UFT	C5-C4	4.24	1.52	1.43
1	A	89	UFT	C5-C4	4.24	1.52	1.43
1	A	197	UFT	C5-C4	4.24	1.52	1.43
1	A	594	CFZ	C2'-C3'	-4.24	1.47	1.52
1	A	90	CFZ	C2'-C3'	-4.24	1.47	1.52
1	A	61	UFT	C5-C4	4.24	1.52	1.43
1	A	547	CFZ	C2'-C3'	-4.23	1.47	1.52
1	A	167	UFT	C5-C4	4.23	1.52	1.43
1	A	263	UFT	C5-C4	4.23	1.52	1.43
1	A	542	UFT	C5-C4	4.23	1.52	1.43
1	A	19	UFT	C2'-C3'	-4.23	1.47	1.52
1	A	705	UFT	C2'-C3'	-4.23	1.47	1.52
1	A	171	CFZ	C2-N3	4.23	1.44	1.36
1	A	538	CFZ	C2-N3	4.23	1.44	1.36
1	A	624	UFT	C5-C4	4.23	1.52	1.43
1	A	23	UFT	C5-C4	4.23	1.52	1.43
1	A	374	UFT	C5-C4	4.23	1.52	1.43
1	A	728	CFZ	C2'-C3'	-4.23	1.47	1.52
1	A	546	CFZ	C2-N3	4.23	1.44	1.36
1	A	431	UFT	C5-C4	4.23	1.52	1.43
1	A	87	CFZ	C2-N3	4.23	1.44	1.36
1	A	559	UFT	C5-C4	4.22	1.52	1.43
1	A	560	CFZ	C2-N3	4.22	1.44	1.36
1	A	23	UFT	C2'-C3'	-4.22	1.47	1.52
1	A	657	CFZ	C2-N3	4.22	1.44	1.36
1	A	590	UFT	C5-C4	4.22	1.52	1.43
1	A	602	CFZ	C2-N3	4.22	1.44	1.36
1	A	182	CFZ	C2-N3	4.22	1.44	1.36
1	A	230	UFT	C5-C4	4.22	1.52	1.43
1	A	157	CFZ	C2-N3	4.22	1.44	1.36
1	A	386	CFZ	C2-N3	4.22	1.44	1.36
1	A	44	UFT	C5-C4	4.21	1.52	1.43
1	A	595	UFT	C5-C4	4.21	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	601	UFT	C5-C4	4.21	1.52	1.43
1	A	17	UFT	C5-C4	4.21	1.52	1.43
1	A	242	UFT	C5-C4	4.21	1.52	1.43
1	A	339	UFT	C5-C4	4.21	1.52	1.43
1	A	409	UFT	C2'-C3'	-4.21	1.47	1.52
1	A	155	CFZ	C2-N3	4.21	1.44	1.36
1	A	493	CFZ	C2-N3	4.21	1.44	1.36
1	A	671	UFT	C5-C4	4.21	1.52	1.43
1	A	275	CFZ	C2-N3	4.21	1.44	1.36
1	A	170	UFT	C5-C4	4.21	1.52	1.43
1	A	699	CFZ	C2-N3	4.21	1.44	1.36
1	A	116	UFT	C5-C4	4.21	1.52	1.43
1	A	120	UFT	C5-C4	4.21	1.52	1.43
1	A	322	UFT	C5-C4	4.21	1.52	1.43
1	A	627	UFT	C5-C4	4.21	1.52	1.43
1	A	612	UFT	C2'-C3'	-4.21	1.47	1.52
1	A	556	UFT	C5-C4	4.21	1.52	1.43
1	A	687	UFT	C2'-C3'	-4.21	1.47	1.52
1	A	377	UFT	C6-N1	4.21	1.48	1.38
1	A	42	UFT	C5-C4	4.21	1.52	1.43
1	A	72	CFZ	C2-N3	4.21	1.44	1.36
1	A	390	UFT	C5-C4	4.20	1.52	1.43
1	A	221	UFT	C5-C4	4.20	1.52	1.43
1	A	230	UFT	C2'-C3'	-4.20	1.47	1.52
1	A	303	UFT	C5-C4	4.20	1.52	1.43
1	A	383	UFT	C5-C4	4.20	1.52	1.43
1	A	564	CFZ	C2-N3	4.20	1.44	1.36
1	A	144	CFZ	C2-N3	4.20	1.44	1.36
1	A	483	CFZ	C2-N3	4.20	1.44	1.36
1	A	523	UFT	C5-C4	4.20	1.52	1.43
1	A	146	CFZ	C2-N3	4.20	1.44	1.36
1	A	95	UFT	C5-C4	4.20	1.52	1.43
1	A	421	UFT	C2'-C3'	-4.20	1.47	1.52
1	A	556	UFT	C2'-C3'	-4.19	1.47	1.52
1	A	360	UFT	C2'-C3'	-4.19	1.47	1.52
1	A	177	UFT	C5-C4	4.19	1.52	1.43
1	A	307	UFT	C5-C4	4.19	1.52	1.43
1	A	638	UFT	C5-C4	4.19	1.52	1.43
1	A	694	CFZ	C2-N3	4.19	1.44	1.36
1	A	267	UFT	C2'-C3'	-4.19	1.47	1.52
1	A	198	CFZ	C2-N3	4.19	1.44	1.36
1	A	485	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	558	UFT	C5-C4	4.19	1.52	1.43
1	A	274	UFT	C5-C4	4.19	1.52	1.43
1	A	409	UFT	C5-C4	4.19	1.52	1.43
1	A	471	UFT	C5-C4	4.19	1.52	1.43
1	A	369	CFZ	C2-N3	4.19	1.44	1.36
1	A	603	CFZ	C2-N3	4.19	1.44	1.36
1	A	236	UFT	C5-C4	4.19	1.52	1.43
1	A	585	UFT	C5-C4	4.19	1.52	1.43
1	A	97	UFT	C5-C4	4.18	1.52	1.43
1	A	272	UFT	C2'-C3'	-4.18	1.47	1.52
1	A	658	CFZ	C2-N3	4.18	1.44	1.36
1	A	288	UFT	C2'-C3'	-4.18	1.47	1.52
1	A	350	UFT	C2'-C3'	-4.18	1.47	1.52
1	A	169	UFT	C5-C4	4.18	1.52	1.43
1	A	46	UFT	C5-C4	4.18	1.52	1.43
1	A	625	CFZ	C2-N3	4.18	1.44	1.36
1	A	283	UFT	C2'-C3'	-4.18	1.47	1.52
1	A	340	UFT	C5-C4	4.18	1.52	1.43
1	A	63	CFZ	C2-N3	4.18	1.44	1.36
1	A	645	CFZ	C2-N3	4.18	1.44	1.36
1	A	468	UFT	C5-C4	4.18	1.52	1.43
1	A	146	CFZ	C2'-C3'	-4.18	1.47	1.52
1	A	339	UFT	C2'-C3'	-4.18	1.47	1.52
1	A	643	UFT	C5-C4	4.17	1.52	1.43
1	A	148	UFT	C5-C4	4.17	1.52	1.43
1	A	724	UFT	C5-C4	4.17	1.52	1.43
1	A	188	UFT	C5-C4	4.17	1.52	1.43
1	A	254	UFT	C5-C4	4.17	1.52	1.43
1	A	97	UFT	C2'-C3'	-4.17	1.47	1.52
1	A	48	UFT	C5-C4	4.17	1.52	1.43
1	A	504	UFT	C5-C4	4.17	1.52	1.43
1	A	26	CFZ	C2-N3	4.17	1.44	1.36
1	A	574	CFZ	C2'-C3'	-4.17	1.47	1.52
1	A	210	UFT	C5-C4	4.16	1.52	1.43
1	A	274	UFT	C2'-C3'	-4.16	1.47	1.52
1	A	500	CFZ	C2'-C3'	-4.16	1.47	1.52
1	A	686	UFT	C2'-C3'	-4.16	1.47	1.52
1	A	383	UFT	C2'-C3'	-4.16	1.47	1.52
1	A	504	UFT	C2'-C3'	-4.16	1.47	1.52
1	A	71	UFT	C5-C4	4.16	1.52	1.43
1	A	81	CFZ	C2-N3	4.16	1.44	1.36
1	A	121	CFZ	C2-N3	4.16	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	UFT	C2'-C3'	-4.16	1.47	1.52
1	A	90	CFZ	C2-N3	4.16	1.44	1.36
1	A	591	CFZ	C2-N3	4.16	1.44	1.36
1	A	687	UFT	C5-C4	4.16	1.52	1.43
1	A	674	CFZ	C2-N3	4.16	1.44	1.36
1	A	128	CFZ	C2'-C3'	-4.15	1.47	1.52
1	A	42	UFT	C2'-C3'	-4.15	1.47	1.52
1	A	521	UFT	C5-C4	4.15	1.52	1.43
1	A	594	CFZ	C2-N3	4.15	1.44	1.36
1	A	360	UFT	C5-C4	4.15	1.52	1.43
1	A	618	CFZ	C2-N3	4.15	1.44	1.36
1	A	6	UFT	C2'-C3'	-4.15	1.47	1.52
1	A	117	CFZ	C2-N3	4.15	1.44	1.36
1	A	507	UFT	C2'-C3'	-4.15	1.47	1.52
1	A	15	CFZ	C2-N3	4.14	1.44	1.36
1	A	192	UFT	C2'-C3'	-4.14	1.47	1.52
1	A	192	UFT	C5-C4	4.14	1.52	1.43
1	A	650	UFT	C5-C4	4.14	1.52	1.43
1	A	194	UFT	C5-C4	4.14	1.52	1.43
1	A	94	UFT	C5-C4	4.14	1.52	1.43
1	A	93	UFT	C5-C4	4.14	1.52	1.43
1	A	641	CFZ	C2-N3	4.14	1.44	1.36
1	A	531	CFZ	C2'-C3'	-4.14	1.47	1.52
1	A	419	UFT	C2'-C3'	-4.14	1.47	1.52
1	A	672	CFZ	C2-N3	4.14	1.44	1.36
1	A	367	UFT	C2'-C3'	-4.14	1.47	1.52
1	A	356	UFT	C5-C4	4.13	1.52	1.43
1	A	502	CFZ	C2-N3	4.13	1.44	1.36
1	A	612	UFT	C5-C4	4.13	1.52	1.43
1	A	370	UFT	C2'-C3'	-4.13	1.47	1.52
1	A	573	UFT	C5-C4	4.12	1.52	1.43
1	A	656	CFZ	C2-N3	4.12	1.44	1.36
1	A	175	UFT	C5-C4	4.12	1.52	1.43
1	A	605	CFZ	C2-N3	4.12	1.44	1.36
1	A	642	UFT	C2'-C3'	-4.12	1.47	1.52
1	A	46	UFT	C2'-C3'	-4.12	1.47	1.52
1	A	94	UFT	C2'-C3'	-4.12	1.47	1.52
1	A	115	UFT	C2'-C3'	-4.12	1.47	1.52
1	A	213	UFT	C2'-C3'	-4.12	1.47	1.52
1	A	390	UFT	C2'-C3'	-4.12	1.47	1.52
1	A	346	CFZ	C2'-C3'	-4.12	1.47	1.52
1	A	574	CFZ	C2-N3	4.12	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	351	UFT	C5-C4	4.12	1.52	1.43
1	A	683	UFT	C5-C4	4.12	1.52	1.43
1	A	188	UFT	C2'-C3'	-4.11	1.47	1.52
1	A	307	UFT	C2'-C3'	-4.11	1.47	1.52
1	A	56	UFT	C5-C4	4.11	1.52	1.43
1	A	506	CFZ	C2-N3	4.11	1.44	1.36
1	A	555	UFT	C5-C4	4.11	1.52	1.43
1	A	361	UFT	C5-C4	4.11	1.52	1.43
1	A	559	UFT	C2'-C3'	-4.11	1.47	1.52
1	A	405	CFZ	C2-N3	4.11	1.44	1.36
1	A	55	CFZ	C2-N3	4.11	1.44	1.36
1	A	419	UFT	C5-C4	4.10	1.52	1.43
1	A	549	UFT	C5-C4	4.10	1.52	1.43
1	A	39	UFT	C2'-C3'	-4.10	1.47	1.52
1	A	585	UFT	C2'-C3'	-4.10	1.47	1.52
1	A	431	UFT	C2'-C3'	-4.10	1.47	1.52
1	A	426	CFZ	C2-N3	4.10	1.44	1.36
1	A	39	UFT	C5-C4	4.10	1.52	1.43
1	A	475	UFT	C5-C4	4.10	1.52	1.43
1	A	627	UFT	C2'-C3'	-4.09	1.47	1.52
1	A	667	UFT	C5-C4	4.09	1.52	1.43
1	A	642	UFT	C5-C4	4.09	1.52	1.43
1	A	193	UFT	C5-C4	4.08	1.52	1.43
1	A	148	UFT	C2'-C3'	-4.08	1.47	1.52
1	A	471	UFT	C2'-C3'	-4.08	1.47	1.52
1	A	550	UFT	C2'-C3'	-4.08	1.47	1.52
1	A	485	UFT	C2'-C3'	-4.08	1.47	1.52
1	A	591	CFZ	C2'-C3'	-4.08	1.47	1.52
1	A	550	UFT	C5-C4	4.08	1.52	1.43
1	A	66	UFT	C5-C4	4.07	1.52	1.43
1	A	374	UFT	C2'-C3'	-4.06	1.47	1.52
1	A	476	UFT	C2'-C3'	-4.06	1.47	1.52
1	A	193	UFT	C2'-C3'	-4.06	1.47	1.52
1	A	181	UFT	C2'-C3'	-4.06	1.47	1.52
1	A	322	UFT	C2'-C3'	-4.06	1.47	1.52
1	A	213	UFT	C5-C4	4.05	1.52	1.43
1	A	329	UFT	C2'-C3'	-4.05	1.47	1.52
1	A	197	UFT	C2'-C3'	-4.05	1.47	1.52
1	A	44	UFT	C2'-C3'	-4.05	1.47	1.52
1	A	662	UFT	C2'-C3'	-4.04	1.47	1.52
1	A	66	UFT	C2'-C3'	-4.04	1.47	1.52
1	A	210	UFT	C2'-C3'	-4.03	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	480	UFT	C2'-C3'	-4.03	1.47	1.52
1	A	371	UFT	C5-C4	4.03	1.52	1.43
1	A	238	UFT	C2'-C3'	-4.02	1.47	1.52
1	A	377	UFT	O4-C4	-4.02	1.16	1.24
1	A	624	UFT	C2'-C3'	-4.02	1.47	1.52
1	A	151	UFT	C2'-C3'	-4.02	1.47	1.52
1	A	33	UFT	C2'-C3'	-4.02	1.47	1.52
1	A	716	UFT	C2'-C3'	-4.01	1.47	1.52
1	A	371	UFT	C2'-C3'	-4.01	1.47	1.52
1	A	717	CFZ	C2'-C3'	-4.01	1.47	1.52
1	A	32	UFT	C2'-C3'	-4.00	1.47	1.52
1	A	215	UFT	C2'-C3'	-4.00	1.47	1.52
1	A	397	UFT	C2'-C3'	-3.99	1.47	1.52
1	A	549	UFT	C2'-C3'	-3.99	1.47	1.52
1	A	670	UFT	C2'-C3'	-3.99	1.47	1.52
1	A	143	UFT	C2'-C3'	-3.99	1.47	1.52
1	A	510	UFT	C2'-C3'	-3.98	1.47	1.52
1	A	444	UFT	C2'-C3'	-3.98	1.47	1.52
1	A	345	UFT	C2'-C3'	-3.97	1.47	1.52
1	A	460	CFZ	C2-N3	3.97	1.44	1.36
1	A	56	UFT	C2'-C3'	-3.96	1.47	1.52
1	A	177	UFT	C2'-C3'	-3.96	1.47	1.52
1	A	574	CFZ	C2'-C1'	-3.96	1.48	1.53
1	A	644	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	597	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	319	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	562	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	638	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	138	UFT	C2'-C3'	-3.95	1.47	1.52
1	A	643	UFT	C2'-C3'	-3.94	1.47	1.52
1	A	167	UFT	C2'-C3'	-3.94	1.47	1.52
1	A	698	UFT	C2'-C3'	-3.94	1.47	1.52
1	A	378	CFZ	C2'-C3'	-3.93	1.47	1.52
1	A	116	UFT	C2'-C3'	-3.92	1.47	1.52
1	A	501	UFT	C2'-C3'	-3.92	1.47	1.52
1	A	590	UFT	C2'-C3'	-3.92	1.47	1.52
1	A	51	UFT	C2'-C3'	-3.91	1.47	1.52
1	A	170	UFT	C2'-C3'	-3.91	1.47	1.52
1	A	532	UFT	C2'-C3'	-3.91	1.47	1.52
1	A	563	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	679	UFT	C2'-C3'	-3.90	1.47	1.52
1	A	88	UFT	C2'-C3'	-3.89	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	UFT	C2'-C3'	-3.89	1.47	1.52
1	A	616	UFT	C2'-C3'	-3.89	1.47	1.52
1	A	194	UFT	C2'-C3'	-3.89	1.47	1.52
1	A	356	UFT	C2'-C3'	-3.88	1.47	1.52
1	A	588	UFT	C2'-C3'	-3.88	1.47	1.52
1	A	34	CFZ	C2'-C3'	-3.87	1.47	1.52
1	A	629	CFZ	C2-N3	3.87	1.44	1.36
1	A	236	UFT	C2'-C3'	-3.87	1.47	1.52
1	A	73	CFZ	C2'-C3'	-3.87	1.47	1.52
1	A	142	UFT	C2'-C3'	-3.87	1.47	1.52
1	A	388	UFT	C2'-C3'	-3.87	1.47	1.52
1	A	542	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	79	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	464	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	523	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	724	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	240	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	377	UFT	C5-C4	3.86	1.52	1.43
1	A	154	UFT	C2'-C3'	-3.86	1.47	1.52
1	A	468	UFT	C2'-C3'	-3.85	1.47	1.52
1	A	123	UFT	C2'-C3'	-3.85	1.47	1.52
1	A	120	UFT	C2'-C3'	-3.85	1.47	1.52
1	A	169	UFT	C2'-C3'	-3.85	1.47	1.52
1	A	351	UFT	C2'-C3'	-3.85	1.47	1.52
1	A	629	CFZ	C2'-C3'	-3.85	1.47	1.52
1	A	242	UFT	C2'-C3'	-3.83	1.47	1.52
1	A	58	UFT	C2'-C3'	-3.83	1.47	1.52
1	A	671	UFT	C2'-C3'	-3.81	1.47	1.52
1	A	719	UFT	C2'-C3'	-3.81	1.47	1.52
1	A	617	UFT	C2'-C3'	-3.81	1.47	1.52
1	A	28	CFZ	O2-C2	3.80	1.30	1.23
1	A	629	CFZ	O2-C2	3.80	1.30	1.23
1	A	303	UFT	C2'-C3'	-3.79	1.47	1.52
1	A	595	UFT	C2'-C3'	-3.79	1.47	1.52
1	A	536	CFZ	C2'-C3'	-3.79	1.47	1.52
1	A	655	UFT	C2'-C3'	-3.78	1.47	1.52
1	A	683	UFT	C2'-C3'	-3.76	1.47	1.52
1	A	531	CFZ	O2-C2	3.75	1.30	1.23
1	A	93	UFT	C2'-C3'	-3.75	1.47	1.52
1	A	706	CFZ	C2'-C3'	-3.73	1.47	1.52
1	A	95	UFT	C2'-C3'	-3.73	1.47	1.52
1	A	473	CFZ	C2'-C3'	-3.73	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	594	CFZ	O2-C2	3.73	1.30	1.23
1	A	536	CFZ	O2-C2	3.72	1.30	1.23
1	A	196	UFT	C2'-C3'	-3.72	1.47	1.52
1	A	379	CFZ	O2-C2	3.71	1.30	1.23
1	A	600	CFZ	O2-C2	3.70	1.30	1.23
1	A	275	CFZ	C2'-C1'	-3.70	1.48	1.53
1	A	277	UFT	C2'-C3'	-3.70	1.47	1.52
1	A	695	CFZ	O2-C2	3.68	1.30	1.23
1	A	493	CFZ	C2'-C1'	-3.68	1.48	1.53
1	A	71	UFT	C2'-C3'	-3.68	1.47	1.52
1	A	713	CFZ	O2-C2	3.68	1.30	1.23
1	A	310	CFZ	C2'-C1'	-3.68	1.48	1.53
1	A	650	UFT	C2'-C3'	-3.68	1.47	1.52
1	A	589	UFT	C2'-C3'	-3.67	1.47	1.52
1	A	717	CFZ	O2-C2	3.67	1.30	1.23
1	A	328	CFZ	O2-C2	3.67	1.30	1.23
1	A	632	CFZ	O2-C2	3.66	1.30	1.23
1	A	416	CFZ	O2-C2	3.66	1.30	1.23
1	A	302	CFZ	C2'-C1'	-3.66	1.48	1.53
1	A	234	CFZ	O2-C2	3.66	1.30	1.23
1	A	62	UFT	C2'-C3'	-3.65	1.47	1.52
1	A	336	CFZ	C2'-C1'	-3.65	1.48	1.53
1	A	667	UFT	C2'-C3'	-3.64	1.47	1.52
1	A	363	CFZ	O2-C2	3.64	1.30	1.23
1	A	484	CFZ	O2-C2	3.63	1.30	1.23
1	A	618	CFZ	O2-C2	3.63	1.30	1.23
1	A	475	UFT	C2'-C3'	-3.63	1.47	1.52
1	A	109	CFZ	O2-C2	3.62	1.30	1.23
1	A	666	CFZ	C2'-C1'	-3.61	1.48	1.53
1	A	526	CFZ	O2-C2	3.61	1.30	1.23
1	A	101	CFZ	O2-C2	3.60	1.30	1.23
1	A	65	CFZ	C2-N3	3.60	1.43	1.36
1	A	369	CFZ	O2-C2	3.60	1.30	1.23
1	A	437	CFZ	O2-C2	3.60	1.30	1.23
1	A	538	CFZ	O2-C2	3.60	1.30	1.23
1	A	490	CFZ	O2-C2	3.60	1.30	1.23
1	A	81	CFZ	O2-C2	3.60	1.30	1.23
1	A	144	CFZ	O2-C2	3.60	1.30	1.23
1	A	217	CFZ	O2-C2	3.60	1.30	1.23
1	A	564	CFZ	O2-C2	3.60	1.30	1.23
1	A	335	CFZ	O2-C2	3.59	1.30	1.23
1	A	57	CFZ	O2-C2	3.59	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	620	CFZ	O2-C2	3.59	1.30	1.23
1	A	117	CFZ	O2-C2	3.59	1.30	1.23
1	A	233	CFZ	O2-C2	3.59	1.30	1.23
1	A	182	CFZ	O2-C2	3.58	1.30	1.23
1	A	108	CFZ	O2-C2	3.58	1.30	1.23
1	A	165	CFZ	O2-C2	3.58	1.30	1.23
1	A	666	CFZ	O2-C2	3.58	1.30	1.23
1	A	613	CFZ	O2-C2	3.58	1.30	1.23
1	A	87	CFZ	O2-C2	3.58	1.30	1.23
1	A	663	CFZ	O2-C2	3.57	1.30	1.23
1	A	382	CFZ	O2-C2	3.57	1.30	1.23
1	A	645	CFZ	O2-C2	3.57	1.30	1.23
1	A	359	CFZ	O2-C2	3.57	1.30	1.23
1	A	512	CFZ	O2-C2	3.57	1.30	1.23
1	A	332	CFZ	O2-C2	3.56	1.30	1.23
1	A	557	CFZ	O2-C2	3.56	1.30	1.23
1	A	55	CFZ	O2-C2	3.56	1.30	1.23
1	A	330	CFZ	O2-C2	3.56	1.30	1.23
1	A	65	CFZ	O2-C2	3.56	1.30	1.23
1	A	273	CFZ	O2-C2	3.56	1.30	1.23
1	A	209	CFZ	O2-C2	3.56	1.30	1.23
1	A	287	CFZ	O2-C2	3.56	1.30	1.23
1	A	198	CFZ	O2-C2	3.56	1.30	1.23
1	A	434	CFZ	O2-C2	3.56	1.30	1.23
1	A	591	CFZ	O2-C2	3.56	1.30	1.23
1	A	727	UFT	C2'-C3'	-3.56	1.48	1.52
1	A	635	CFZ	O2-C2	3.56	1.30	1.23
1	A	649	CFZ	C2'-C1'	-3.56	1.48	1.53
1	A	90	CFZ	O2-C2	3.55	1.30	1.23
1	A	10	CFZ	O2-C2	3.55	1.30	1.23
1	A	50	CFZ	C2'-C1'	-3.55	1.48	1.53
1	A	63	CFZ	O2-C2	3.55	1.30	1.23
1	A	83	CFZ	O2-C2	3.55	1.30	1.23
1	A	130	CFZ	O2-C2	3.55	1.30	1.23
1	A	146	CFZ	O2-C2	3.55	1.30	1.23
1	A	12	CFZ	O2-C2	3.55	1.30	1.23
1	A	83	CFZ	O4'-C1'	3.54	1.50	1.42
1	A	499	CFZ	O2-C2	3.54	1.30	1.23
1	A	637	CFZ	O2-C2	3.54	1.30	1.23
1	A	378	CFZ	O2-C2	3.54	1.30	1.23
1	A	212	CFZ	O2-C2	3.54	1.30	1.23
1	A	466	CFZ	O2-C2	3.54	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	CFZ	O2-C2	3.54	1.30	1.23
1	A	344	CFZ	O2-C2	3.54	1.30	1.23
1	A	72	CFZ	O2-C2	3.54	1.30	1.23
1	A	675	CFZ	O2-C2	3.54	1.30	1.23
1	A	658	CFZ	O2-C2	3.54	1.30	1.23
1	A	706	CFZ	O2-C2	3.54	1.30	1.23
1	A	276	CFZ	O2-C2	3.53	1.30	1.23
1	A	190	CFZ	O2-C2	3.53	1.30	1.23
1	A	574	CFZ	O2-C2	3.53	1.30	1.23
1	A	674	CFZ	O2-C2	3.53	1.30	1.23
1	A	244	CFZ	O2-C2	3.53	1.30	1.23
1	A	395	CFZ	O2-C2	3.53	1.30	1.23
1	A	156	CFZ	O2-C2	3.53	1.30	1.23
1	A	522	CFZ	O2-C2	3.53	1.30	1.23
1	A	672	CFZ	O2-C2	3.53	1.30	1.23
1	A	631	CFZ	O2-C2	3.53	1.30	1.23
1	A	600	CFZ	C2'-C1'	-3.53	1.48	1.53
1	A	336	CFZ	O2-C2	3.53	1.30	1.23
1	A	310	CFZ	O2-C2	3.52	1.30	1.23
1	A	34	CFZ	O2-C2	3.52	1.30	1.23
1	A	439	CFZ	O2-C2	3.52	1.30	1.23
1	A	147	CFZ	O2-C2	3.52	1.30	1.23
1	A	699	CFZ	O2-C2	3.52	1.30	1.23
1	A	625	CFZ	O2-C2	3.52	1.30	1.23
1	A	137	CFZ	O2-C2	3.52	1.30	1.23
1	A	391	CFZ	O2-C2	3.52	1.30	1.23
1	A	128	CFZ	O2-C2	3.52	1.30	1.23
1	A	500	CFZ	O2-C2	3.52	1.30	1.23
1	A	173	CFZ	O2-C2	3.52	1.30	1.23
1	A	515	CFZ	O2-C2	3.52	1.30	1.23
1	A	111	CFZ	O2-C2	3.51	1.30	1.23
1	A	690	CFZ	O2-C2	3.51	1.30	1.23
1	A	685	CFZ	O2-C2	3.51	1.30	1.23
1	A	114	CFZ	O2-C2	3.51	1.30	1.23
1	A	45	CFZ	O2-C2	3.51	1.30	1.23
1	A	50	CFZ	O2-C2	3.51	1.30	1.23
1	A	256	CFZ	O2-C2	3.51	1.30	1.23
1	A	219	CFZ	O2-C2	3.51	1.30	1.23
1	A	343	CFZ	O2-C2	3.51	1.30	1.23
1	A	665	CFZ	O2-C2	3.51	1.30	1.23
1	A	337	CFZ	O2-C2	3.51	1.30	1.23
1	A	384	CFZ	O2-C2	3.51	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	438	CFZ	O2-C2	3.51	1.30	1.23
1	A	11	CFZ	O2-C2	3.50	1.30	1.23
1	A	342	CFZ	O2-C2	3.50	1.30	1.23
1	A	463	CFZ	O2-C2	3.50	1.30	1.23
1	A	604	CFZ	O2-C2	3.50	1.30	1.23
1	A	271	CFZ	O2-C2	3.50	1.30	1.23
1	A	577	CFZ	O2-C2	3.50	1.30	1.23
1	A	76	CFZ	O2-C2	3.50	1.30	1.23
1	A	661	CFZ	O2-C2	3.50	1.30	1.23
1	A	561	CFZ	O2-C2	3.50	1.30	1.23
1	A	171	CFZ	O2-C2	3.50	1.30	1.23
1	A	17	UFT	C2'-C3'	-3.50	1.48	1.52
1	A	453	CFZ	O2-C2	3.50	1.30	1.23
1	A	432	CFZ	O2-C2	3.50	1.30	1.23
1	A	162	CFZ	O2-C2	3.50	1.30	1.23
1	A	696	CFZ	O2-C2	3.50	1.30	1.23
1	A	458	CFZ	O2-C2	3.49	1.30	1.23
1	A	184	CFZ	O2-C2	3.49	1.30	1.23
1	A	709	CFZ	O2-C2	3.49	1.30	1.23
1	A	206	CFZ	O2-C2	3.49	1.30	1.23
1	A	155	CFZ	O2-C2	3.49	1.30	1.23
1	A	489	CFZ	O2-C2	3.49	1.30	1.23
1	A	7	CFZ	O2-C2	3.49	1.30	1.23
1	A	547	CFZ	O2-C2	3.48	1.30	1.23
1	A	147	CFZ	C2'-C1'	-3.48	1.48	1.53
1	A	630	CFZ	O2-C2	3.48	1.30	1.23
1	A	433	CFZ	O2-C2	3.48	1.30	1.23
1	A	73	CFZ	O2-C2	3.48	1.30	1.23
1	A	45	CFZ	C2'-C1'	-3.48	1.48	1.53
1	A	602	CFZ	O2-C2	3.48	1.30	1.23
1	A	153	CFZ	O2-C2	3.48	1.30	1.23
1	A	694	CFZ	O2-C2	3.48	1.30	1.23
1	A	487	CFZ	O2-C2	3.48	1.30	1.23
1	A	129	CFZ	O2-C2	3.47	1.30	1.23
1	A	641	CFZ	O2-C2	3.47	1.30	1.23
1	A	598	CFZ	O2-C2	3.47	1.30	1.23
1	A	75	CFZ	O2-C2	3.47	1.30	1.23
1	A	422	CFZ	O2-C2	3.47	1.30	1.23
1	A	502	CFZ	O2-C2	3.47	1.30	1.23
1	A	195	CFZ	O2-C2	3.47	1.30	1.23
1	A	135	CFZ	O2-C2	3.46	1.30	1.23
1	A	407	CFZ	O2-C2	3.46	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	CFZ	O2-C2	3.46	1.30	1.23
1	A	26	CFZ	O2-C2	3.46	1.30	1.23
1	A	103	CFZ	O2-C2	3.46	1.30	1.23
1	A	609	CFZ	O2-C2	3.46	1.30	1.23
1	A	161	CFZ	O2-C2	3.46	1.30	1.23
1	A	728	CFZ	O2-C2	3.46	1.30	1.23
1	A	366	CFZ	O2-C2	3.46	1.30	1.23
1	A	653	CFZ	O2-C2	3.46	1.30	1.23
1	A	41	CFZ	O2-C2	3.45	1.30	1.23
1	A	306	CFZ	O2-C2	3.45	1.30	1.23
1	A	442	CFZ	O2-C2	3.45	1.30	1.23
1	A	137	CFZ	C2'-C1'	-3.45	1.48	1.53
1	A	121	CFZ	O2-C2	3.45	1.30	1.23
1	A	649	CFZ	O2-C2	3.45	1.30	1.23
1	A	467	CFZ	O2-C2	3.45	1.30	1.23
1	A	720	CFZ	O2-C2	3.45	1.30	1.23
1	A	518	CFZ	C2'-C1'	-3.45	1.48	1.53
1	A	518	CFZ	O2-C2	3.44	1.30	1.23
1	A	605	CFZ	O2-C2	3.44	1.30	1.23
1	A	541	CFZ	O2-C2	3.44	1.30	1.23
1	A	337	CFZ	O4'-C1'	3.44	1.49	1.42
1	A	506	CFZ	O2-C2	3.44	1.30	1.23
1	A	363	CFZ	O4'-C1'	3.44	1.49	1.42
1	A	269	CFZ	O2-C2	3.44	1.30	1.23
1	A	657	CFZ	O2-C2	3.44	1.30	1.23
1	A	452	CFZ	O2-C2	3.44	1.30	1.23
1	A	392	CFZ	O2-C2	3.44	1.30	1.23
1	A	603	CFZ	O2-C2	3.44	1.30	1.23
1	A	456	CFZ	O2-C2	3.44	1.30	1.23
1	A	689	CFZ	O2-C2	3.44	1.30	1.23
1	A	28	CFZ	O4'-C1'	3.43	1.49	1.42
1	A	175	UFT	C2'-C3'	-3.43	1.48	1.52
1	A	291	CFZ	O2-C2	3.43	1.30	1.23
1	A	83	CFZ	C2'-C1'	-3.43	1.49	1.53
1	A	80	CFZ	O2-C2	3.43	1.30	1.23
1	A	426	CFZ	O2-C2	3.43	1.30	1.23
1	A	473	CFZ	O2-C2	3.43	1.30	1.23
1	A	656	CFZ	O2-C2	3.43	1.30	1.23
1	A	362	CFZ	O2-C2	3.43	1.30	1.23
1	A	89	UFT	C2'-C3'	-3.42	1.48	1.52
1	A	346	CFZ	O2-C2	3.42	1.30	1.23
1	A	104	CFZ	O2-C2	3.42	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	CFZ	O2-C2	3.42	1.30	1.23
1	A	527	CFZ	O2-C2	3.42	1.30	1.23
1	A	153	CFZ	C2'-C1'	-3.42	1.49	1.53
1	A	308	CFZ	O2-C2	3.42	1.30	1.23
1	A	314	CFZ	O2-C2	3.41	1.30	1.23
1	A	204	CFZ	O2-C2	3.41	1.30	1.23
1	A	706	CFZ	O4'-C1'	3.41	1.49	1.42
1	A	178	CFZ	O2-C2	3.41	1.30	1.23
1	A	536	CFZ	O4'-C1'	3.41	1.49	1.42
1	A	15	CFZ	O2-C2	3.41	1.30	1.23
1	A	546	CFZ	O2-C2	3.40	1.30	1.23
1	A	127	UFT	C2'-C3'	-3.40	1.48	1.52
1	A	275	CFZ	O2-C2	3.40	1.30	1.23
1	A	72	CFZ	C2'-C1'	-3.40	1.49	1.53
1	A	386	CFZ	O2-C2	3.40	1.30	1.23
1	A	28	CFZ	C2'-C3'	-3.39	1.48	1.52
1	A	276	CFZ	C2'-C1'	-3.39	1.49	1.53
1	A	483	CFZ	O2-C2	3.39	1.30	1.23
1	A	697	UFT	C2'-C3'	-3.39	1.48	1.52
1	A	493	CFZ	O2-C2	3.39	1.30	1.23
1	A	157	CFZ	O2-C2	3.39	1.30	1.23
1	A	560	CFZ	O2-C2	3.39	1.30	1.23
1	A	473	CFZ	O4'-C1'	3.38	1.49	1.42
1	A	332	CFZ	C2'-C1'	-3.38	1.49	1.53
1	A	709	CFZ	O4'-C1'	3.38	1.49	1.42
1	A	335	CFZ	C2'-C1'	-3.38	1.49	1.53
1	A	557	CFZ	C2'-C1'	-3.38	1.49	1.53
1	A	384	CFZ	O4'-C1'	3.38	1.49	1.42
1	A	625	CFZ	O4'-C1'	3.38	1.49	1.42
1	A	308	CFZ	C2'-C1'	-3.38	1.49	1.53
1	A	621	CFZ	O2-C2	3.38	1.30	1.23
1	A	209	CFZ	C2'-C1'	-3.37	1.49	1.53
1	A	256	CFZ	C2'-C1'	-3.37	1.49	1.53
1	A	629	CFZ	O4'-C1'	3.37	1.49	1.42
1	A	328	CFZ	O4'-C1'	3.37	1.49	1.42
1	A	131	CFZ	O2-C2	3.37	1.30	1.23
1	A	302	CFZ	O2-C2	3.37	1.30	1.23
1	A	487	CFZ	O4'-C1'	3.37	1.49	1.42
1	A	594	CFZ	O4'-C1'	3.36	1.49	1.42
1	A	366	CFZ	O4'-C1'	3.36	1.49	1.42
1	A	471	UFT	C2'-C1'	-3.36	1.49	1.53
1	A	51	UFT	C2'-C1'	-3.36	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	CFZ	C2'-C1'	-3.36	1.49	1.53
1	A	7	CFZ	O4'-C1'	3.35	1.49	1.42
1	A	379	CFZ	O4'-C1'	3.35	1.49	1.42
1	A	434	CFZ	O4'-C1'	3.35	1.49	1.42
1	A	600	CFZ	O4'-C1'	3.35	1.49	1.42
1	A	484	CFZ	O4'-C1'	3.35	1.49	1.42
1	A	632	CFZ	O4'-C1'	3.34	1.49	1.42
1	A	213	UFT	C2'-C1'	-3.34	1.49	1.53
1	A	675	CFZ	C2'-C1'	-3.34	1.49	1.53
1	A	57	CFZ	C2'-C1'	-3.34	1.49	1.53
1	A	515	CFZ	O4'-C1'	3.34	1.49	1.42
1	A	219	CFZ	C2'-C1'	-3.34	1.49	1.53
1	A	518	CFZ	O4'-C1'	3.33	1.49	1.42
1	A	657	CFZ	C2'-C1'	-3.33	1.49	1.53
1	A	75	CFZ	O4'-C1'	3.32	1.49	1.42
1	A	541	CFZ	C2'-C1'	-3.32	1.49	1.53
1	A	395	CFZ	O4'-C1'	3.32	1.49	1.42
1	A	620	CFZ	O4'-C1'	3.32	1.49	1.42
1	A	103	CFZ	O4'-C1'	3.32	1.49	1.42
1	A	306	CFZ	C2'-C1'	-3.32	1.49	1.53
1	A	490	CFZ	O4'-C1'	3.32	1.49	1.42
1	A	103	CFZ	C2'-C1'	-3.32	1.49	1.53
1	A	276	CFZ	O4'-C1'	3.31	1.49	1.42
1	A	362	CFZ	C2'-C1'	-3.31	1.49	1.53
1	A	416	CFZ	O4'-C1'	3.31	1.49	1.42
1	A	499	CFZ	C2'-C1'	-3.31	1.49	1.53
1	A	463	CFZ	O4'-C1'	3.31	1.49	1.42
1	A	311	UFT	C2'-C1'	-3.30	1.49	1.53
1	A	41	CFZ	O4'-C1'	3.30	1.49	1.42
1	A	439	CFZ	O4'-C1'	3.30	1.49	1.42
1	A	332	CFZ	O4'-C1'	3.30	1.49	1.42
1	A	466	CFZ	C2'-C1'	-3.30	1.49	1.53
1	A	437	CFZ	C2'-C1'	-3.30	1.49	1.53
1	A	121	CFZ	O4'-C1'	3.30	1.49	1.42
1	A	330	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	422	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	336	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	604	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	342	CFZ	C2'-C1'	-3.29	1.49	1.53
1	A	72	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	108	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	452	CFZ	O4'-C1'	3.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	561	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	343	CFZ	C2'-C1'	-3.29	1.49	1.53
1	A	541	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	434	CFZ	C2'-C1'	-3.29	1.49	1.53
1	A	135	CFZ	O4'-C1'	3.29	1.49	1.42
1	A	437	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	453	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	695	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	522	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	713	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	129	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	109	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	557	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	489	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	382	CFZ	O4'-C1'	3.28	1.49	1.42
1	A	217	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	80	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	302	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	432	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	620	CFZ	C2'-C1'	-3.27	1.49	1.53
1	A	689	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	560	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	577	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	696	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	310	CFZ	O4'-C1'	3.27	1.49	1.42
1	A	213	UFT	O4-C4	-3.27	1.18	1.24
1	A	198	CFZ	C2'-C1'	-3.27	1.49	1.53
1	A	405	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	198	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	342	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	452	CFZ	C2'-C1'	-3.26	1.49	1.53
1	A	209	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	460	CFZ	O2-C2	3.26	1.29	1.23
1	A	81	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	369	CFZ	C2'-C1'	-3.26	1.49	1.53
1	A	161	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	55	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	308	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	343	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	344	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	604	CFZ	C2'-C1'	-3.26	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	456	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	598	CFZ	O4'-C1'	3.26	1.49	1.42
1	A	594	CFZ	C2'-C1'	-3.25	1.49	1.53
1	A	314	CFZ	O4'-C1'	3.25	1.49	1.42
1	A	190	CFZ	O4'-C1'	3.25	1.49	1.42
1	A	382	CFZ	C2'-C1'	-3.25	1.49	1.53
1	A	130	CFZ	O4'-C1'	3.25	1.49	1.42
1	A	649	CFZ	O4'-C1'	3.25	1.49	1.42
1	A	12	CFZ	O4'-C1'	3.25	1.49	1.42
1	A	162	CFZ	O4'-C1'	3.25	1.49	1.42
1	A	538	CFZ	O4'-C1'	3.25	1.49	1.42
1	A	291	CFZ	O4'-C1'	3.25	1.49	1.42
1	A	173	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	147	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	287	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	87	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	234	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	426	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	546	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	635	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	212	CFZ	C2'-C1'	-3.24	1.49	1.53
1	A	512	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	182	CFZ	C2'-C1'	-3.24	1.49	1.53
1	A	609	CFZ	O4'-C1'	3.24	1.49	1.42
1	A	34	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	526	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	369	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	663	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	137	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	433	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	653	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	76	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	114	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	484	CFZ	C2'-C1'	-3.23	1.49	1.53
1	A	466	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	66	UFT	C2'-C1'	-3.23	1.49	1.53
1	A	275	CFZ	O4'-C1'	3.23	1.49	1.42
1	A	111	CFZ	C2'-C1'	-3.23	1.49	1.53
1	A	407	CFZ	C2'-C1'	-3.22	1.49	1.53
1	A	111	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	467	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	522	CFZ	C2'-C1'	-3.22	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	104	CFZ	C2'-C1'	-3.22	1.49	1.53
1	A	104	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	212	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	273	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	10	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	195	CFZ	C2'-C1'	-3.22	1.49	1.53
1	A	458	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	506	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	613	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	57	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	269	CFZ	O4'-C1'	3.22	1.49	1.42
1	A	11	CFZ	O4'-C1'	3.21	1.49	1.42
1	A	531	CFZ	O4'-C1'	3.21	1.49	1.42
1	A	165	CFZ	O4'-C1'	3.21	1.49	1.42
1	A	184	CFZ	O4'-C1'	3.21	1.49	1.42
1	A	233	CFZ	O4'-C1'	3.21	1.49	1.42
1	A	156	CFZ	O4'-C1'	3.21	1.49	1.42
1	A	65	CFZ	O4'-C1'	3.21	1.49	1.42
1	A	578	CFZ	O4'-C1'	3.21	1.49	1.42
1	A	547	CFZ	O4'-C1'	3.21	1.49	1.42
1	A	204	CFZ	C2'-C1'	-3.21	1.49	1.53
1	A	208	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	359	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	439	CFZ	C2'-C1'	-3.20	1.49	1.53
1	A	204	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	346	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	178	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	605	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	728	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	546	CFZ	C2'-C1'	-3.20	1.49	1.53
1	A	244	CFZ	O4'-C1'	3.20	1.49	1.42
1	A	602	CFZ	C2'-C1'	-3.20	1.49	1.53
1	A	442	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	190	CFZ	C2'-C1'	-3.19	1.49	1.53
1	A	66	UFT	O4-C4	-3.19	1.18	1.24
1	A	371	UFT	O4-C4	-3.19	1.18	1.24
1	A	485	UFT	C2'-C1'	-3.19	1.49	1.53
1	A	386	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	157	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	195	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	34	CFZ	C2'-C1'	-3.19	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	CFZ	C2'-C1'	-3.19	1.49	1.53
1	A	602	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	337	CFZ	C2'-C1'	-3.19	1.49	1.53
1	A	631	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	362	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	641	CFZ	O4'-C1'	3.19	1.49	1.42
1	A	577	CFZ	C2'-C1'	-3.18	1.49	1.53
1	A	219	CFZ	O4'-C1'	3.18	1.49	1.42
1	A	499	CFZ	O4'-C1'	3.18	1.49	1.42
1	A	422	CFZ	C2'-C1'	-3.18	1.49	1.53
1	A	531	CFZ	C2'-C1'	-3.18	1.49	1.53
1	A	344	CFZ	C2'-C1'	-3.17	1.49	1.53
1	A	460	CFZ	C2'-C1'	-3.17	1.49	1.53
1	A	690	CFZ	O4'-C1'	3.17	1.49	1.42
1	A	650	UFT	O4-C4	-3.17	1.18	1.24
1	A	366	CFZ	C2'-C1'	-3.17	1.49	1.53
1	A	665	CFZ	O4'-C1'	3.17	1.49	1.42
1	A	672	CFZ	C2'-C1'	-3.17	1.49	1.53
1	A	101	CFZ	O4'-C1'	3.17	1.49	1.42
1	A	153	CFZ	O4'-C1'	3.16	1.49	1.42
1	A	131	CFZ	O4'-C1'	3.16	1.49	1.42
1	A	146	CFZ	C2'-C1'	-3.16	1.49	1.53
1	A	666	CFZ	O4'-C1'	3.16	1.49	1.42
1	A	661	CFZ	O4'-C1'	3.16	1.49	1.42
1	A	12	CFZ	C2'-C1'	-3.16	1.49	1.53
1	A	306	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	392	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	637	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	50	CFZ	O4'-C1'	3.15	1.49	1.42
1	A	184	CFZ	C2'-C1'	-3.15	1.49	1.53
1	A	26	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	271	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	694	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	717	CFZ	C2'-C1'	-3.14	1.49	1.53
1	A	493	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	483	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	15	CFZ	O4'-C1'	3.14	1.49	1.42
1	A	144	CFZ	C2'-C1'	-3.13	1.49	1.53
1	A	601	UFT	C2'-C3'	-3.13	1.48	1.52
1	A	621	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	717	CFZ	O4'-C1'	3.13	1.49	1.42
1	A	521	UFT	C2'-C1'	-3.13	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	500	CFZ	C2'-C1'	-3.13	1.49	1.53
1	A	7	CFZ	C2'-C1'	-3.13	1.49	1.53
1	A	63	CFZ	C2'-C1'	-3.13	1.49	1.53
1	A	433	CFZ	C2'-C1'	-3.12	1.49	1.53
1	A	658	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	632	CFZ	C2'-C1'	-3.12	1.49	1.53
1	A	244	CFZ	C2'-C1'	-3.12	1.49	1.53
1	A	720	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	256	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	630	CFZ	O4'-C1'	3.12	1.49	1.42
1	A	335	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	665	CFZ	C2'-C1'	-3.11	1.49	1.53
1	A	489	CFZ	C2'-C1'	-3.11	1.49	1.53
1	A	210	UFT	O4-C4	-3.11	1.18	1.24
1	A	273	CFZ	C2'-C1'	-3.11	1.49	1.53
1	A	378	CFZ	O4'-C1'	3.11	1.49	1.42
1	A	467	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	527	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	675	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	73	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	128	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	453	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	656	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	355	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	536	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	527	CFZ	O4'-C1'	3.10	1.49	1.42
1	A	130	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	165	CFZ	C2'-C1'	-3.10	1.49	1.53
1	A	287	CFZ	C2'-C1'	-3.09	1.49	1.53
1	A	667	UFT	C2'-C1'	-3.08	1.49	1.53
1	A	674	CFZ	C2'-C1'	-3.08	1.49	1.53
1	A	694	CFZ	C2'-C1'	-3.08	1.49	1.53
1	A	574	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	699	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	547	CFZ	C2'-C1'	-3.08	1.49	1.53
1	A	683	UFT	O4-C4	-3.08	1.18	1.24
1	A	685	CFZ	O4'-C1'	3.08	1.49	1.42
1	A	613	CFZ	C2'-C1'	-3.08	1.49	1.53
1	A	194	UFT	O4-C4	-3.07	1.18	1.24
1	A	442	CFZ	C2'-C1'	-3.07	1.49	1.53
1	A	329	UFT	C2'-C1'	-3.07	1.49	1.53
1	A	63	CFZ	O4'-C1'	3.07	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	CFZ	C2'-C1'	-3.07	1.49	1.53
1	A	10	CFZ	C2'-C1'	-3.06	1.49	1.53
1	A	578	CFZ	O2-C2	3.06	1.29	1.23
1	A	155	CFZ	O4'-C1'	3.06	1.49	1.42
1	A	87	CFZ	C2'-C1'	-3.06	1.49	1.53
1	A	384	CFZ	C2'-C1'	-3.06	1.49	1.53
1	A	182	CFZ	O4'-C1'	3.06	1.49	1.42
1	A	65	CFZ	C2'-C1'	-3.06	1.49	1.53
1	A	603	CFZ	O4'-C1'	3.05	1.49	1.42
1	A	117	CFZ	O4'-C1'	3.05	1.49	1.42
1	A	674	CFZ	O4'-C1'	3.05	1.49	1.42
1	A	391	CFZ	O4'-C1'	3.05	1.49	1.42
1	A	374	UFT	O4-C4	-3.05	1.18	1.24
1	A	645	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	603	CFZ	C2'-C1'	-3.04	1.49	1.53
1	A	128	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	687	UFT	O4-C4	-3.04	1.18	1.24
1	A	629	CFZ	C2'-C1'	-3.04	1.49	1.53
1	A	538	CFZ	C2'-C1'	-3.04	1.49	1.53
1	A	206	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	591	CFZ	C2'-C1'	-3.04	1.49	1.53
1	A	483	CFZ	C2'-C1'	-3.04	1.49	1.53
1	A	618	CFZ	O4'-C1'	3.04	1.49	1.42
1	A	564	CFZ	C2'-C1'	-3.04	1.49	1.53
1	A	51	UFT	O4-C4	-3.03	1.18	1.24
1	A	605	CFZ	C2'-C1'	-3.03	1.49	1.53
1	A	109	CFZ	C2'-C1'	-3.03	1.49	1.53
1	A	171	CFZ	O4'-C1'	3.03	1.49	1.42
1	A	625	CFZ	C2'-C1'	-3.03	1.49	1.53
1	A	101	CFZ	C2'-C1'	-3.03	1.49	1.53
1	A	236	UFT	C2'-C1'	-3.03	1.49	1.53
1	A	656	CFZ	O4'-C1'	3.03	1.49	1.42
1	A	416	CFZ	C2'-C1'	-3.03	1.49	1.53
1	A	560	CFZ	C2'-C1'	-3.03	1.49	1.53
1	A	635	CFZ	C2'-C1'	-3.03	1.49	1.53
1	A	73	CFZ	O4'-C1'	3.02	1.49	1.42
1	A	56	UFT	O4-C4	-3.02	1.18	1.24
1	A	696	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	631	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	90	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	645	CFZ	C2'-C1'	-3.02	1.49	1.53
1	A	609	CFZ	C2'-C1'	-3.02	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	391	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	208	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	661	CFZ	C2'-C1'	-3.01	1.49	1.53
1	A	367	UFT	O4-C4	-3.00	1.18	1.24
1	A	706	CFZ	C2'-C1'	-3.00	1.49	1.53
1	A	504	UFT	O4-C4	-3.00	1.18	1.24
1	A	438	CFZ	O4'-C1'	3.00	1.48	1.42
1	A	724	UFT	C2'-C1'	-3.00	1.49	1.53
1	A	612	UFT	O4-C4	-3.00	1.18	1.24
1	A	407	CFZ	O4'-C1'	3.00	1.48	1.42
1	A	720	CFZ	C2'-C1'	-3.00	1.49	1.53
1	A	213	UFT	C2-N3	3.00	1.43	1.38
1	A	638	UFT	O4-C4	-2.99	1.18	1.24
1	A	236	UFT	O4-C4	-2.99	1.18	1.24
1	A	233	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	658	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	93	UFT	O4-C4	-2.99	1.18	1.24
1	A	515	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	460	CFZ	O4'-C1'	2.99	1.48	1.42
1	A	192	UFT	O4-C4	-2.99	1.18	1.24
1	A	291	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	695	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	193	UFT	O4-C4	-2.99	1.18	1.24
1	A	58	UFT	C2'-C1'	-2.99	1.49	1.53
1	A	162	CFZ	C2'-C1'	-2.99	1.49	1.53
1	A	363	CFZ	C2'-C1'	-2.98	1.49	1.53
1	A	15	CFZ	C2'-C1'	-2.98	1.49	1.53
1	A	144	CFZ	O4'-C1'	2.98	1.48	1.42
1	A	591	CFZ	O4'-C1'	2.98	1.48	1.42
1	A	42	UFT	O4-C4	-2.98	1.18	1.24
1	A	390	UFT	O4-C4	-2.98	1.18	1.24
1	A	650	UFT	C2-N3	2.98	1.43	1.38
1	A	148	UFT	O4-C4	-2.98	1.18	1.24
1	A	728	CFZ	C2'-C1'	-2.98	1.49	1.53
1	A	549	UFT	O4-C4	-2.97	1.18	1.24
1	A	76	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	657	CFZ	O4'-C1'	2.97	1.48	1.42
1	A	155	CFZ	C2'-C1'	-2.97	1.49	1.53
1	A	210	UFT	C2-N3	2.97	1.43	1.38
1	A	476	UFT	O4-C4	-2.97	1.18	1.24
1	A	120	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	80	CFZ	C2'-C1'	-2.96	1.49	1.53
1	A	55	CFZ	C2'-C1'	-2.96	1.49	1.53
1	A	175	UFT	O4-C4	-2.96	1.18	1.24
1	A	242	UFT	O4-C4	-2.96	1.18	1.24
1	A	607	UFT	O4-C4	-2.96	1.18	1.24
1	A	637	CFZ	C2'-C1'	-2.96	1.49	1.53
1	A	107	UFT	O4-C4	-2.96	1.18	1.24
1	A	356	UFT	O4-C4	-2.95	1.18	1.24
1	A	94	UFT	O4-C4	-2.95	1.18	1.24
1	A	598	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	370	UFT	O4-C4	-2.95	1.18	1.24
1	A	263	UFT	O4-C4	-2.95	1.18	1.24
1	A	542	UFT	O4-C4	-2.95	1.18	1.24
1	A	616	UFT	O4-C4	-2.95	1.18	1.24
1	A	502	CFZ	O4'-C1'	2.95	1.48	1.42
1	A	97	UFT	C2'-C1'	-2.95	1.49	1.53
1	A	558	UFT	C2'-C1'	-2.95	1.49	1.53
1	A	23	UFT	O4-C4	-2.95	1.18	1.24
1	A	196	UFT	O4-C4	-2.95	1.18	1.24
1	A	601	UFT	O4-C4	-2.95	1.18	1.24
1	A	558	UFT	O4-C4	-2.95	1.18	1.24
1	A	563	UFT	O4-C4	-2.95	1.18	1.24
1	A	473	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	114	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	512	CFZ	C2'-C1'	-2.95	1.49	1.53
1	A	612	UFT	C2'-C1'	-2.95	1.49	1.53
1	A	173	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	33	UFT	O4-C4	-2.94	1.18	1.24
1	A	142	UFT	O4-C4	-2.94	1.18	1.24
1	A	627	UFT	O4-C4	-2.94	1.18	1.24
1	A	630	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	340	UFT	O4-C4	-2.94	1.18	1.24
1	A	471	UFT	O4-C4	-2.94	1.18	1.24
1	A	117	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	679	UFT	O4-C4	-2.94	1.18	1.24
1	A	361	UFT	C2'-C1'	-2.94	1.49	1.53
1	A	642	UFT	O4-C4	-2.94	1.18	1.24
1	A	507	UFT	O4-C4	-2.94	1.18	1.24
1	A	464	UFT	O4-C4	-2.94	1.18	1.24
1	A	575	UFT	O4-C4	-2.94	1.18	1.24
1	A	624	UFT	O4-C4	-2.94	1.18	1.24
1	A	667	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	502	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	330	CFZ	C2'-C1'	-2.94	1.49	1.53
1	A	303	UFT	O4-C4	-2.93	1.18	1.24
1	A	550	UFT	O4-C4	-2.93	1.18	1.24
1	A	468	UFT	O4-C4	-2.93	1.18	1.24
1	A	329	UFT	O4-C4	-2.93	1.18	1.24
1	A	419	UFT	O4-C4	-2.93	1.18	1.24
1	A	88	UFT	O4-C4	-2.93	1.18	1.24
1	A	559	UFT	O4-C4	-2.93	1.18	1.24
1	A	6	UFT	O4-C4	-2.93	1.18	1.24
1	A	267	UFT	O4-C4	-2.93	1.18	1.24
1	A	90	CFZ	O4'-C1'	2.93	1.48	1.42
1	A	127	UFT	O4-C4	-2.93	1.18	1.24
1	A	339	UFT	O4-C4	-2.93	1.18	1.24
1	A	167	UFT	O4-C4	-2.93	1.18	1.24
1	A	97	UFT	O4-C4	-2.93	1.18	1.24
1	A	361	UFT	O4-C4	-2.93	1.18	1.24
1	A	44	UFT	C2'-C1'	-2.92	1.49	1.53
1	A	643	UFT	O4-C4	-2.92	1.18	1.24
1	A	689	CFZ	C2'-C1'	-2.92	1.49	1.53
1	A	66	UFT	C2-N3	2.92	1.43	1.38
1	A	288	UFT	O4-C4	-2.92	1.18	1.24
1	A	617	UFT	O4-C4	-2.92	1.18	1.24
1	A	314	CFZ	C2'-C1'	-2.92	1.49	1.53
1	A	699	CFZ	C2'-C1'	-2.92	1.49	1.53
1	A	32	UFT	O4-C4	-2.92	1.18	1.24
1	A	361	UFT	C2'-C3'	-2.92	1.48	1.52
1	A	277	UFT	O4-C4	-2.92	1.18	1.24
1	A	345	UFT	C2'-C1'	-2.92	1.49	1.53
1	A	46	UFT	O4-C4	-2.91	1.18	1.24
1	A	359	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	156	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	367	UFT	C2-N3	2.91	1.43	1.38
1	A	421	UFT	O4-C4	-2.91	1.18	1.24
1	A	653	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	48	UFT	O4-C4	-2.91	1.18	1.24
1	A	61	UFT	O4-C4	-2.91	1.18	1.24
1	A	641	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	388	UFT	O4-C4	-2.91	1.18	1.24
1	A	44	UFT	O4-C4	-2.91	1.18	1.24
1	A	697	UFT	O4-C4	-2.91	1.18	1.24
1	A	360	UFT	O4-C4	-2.91	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	556	UFT	O4-C4	-2.91	1.18	1.24
1	A	644	UFT	O4-C4	-2.91	1.18	1.24
1	A	595	UFT	O4-C4	-2.91	1.18	1.24
1	A	618	CFZ	C2'-C1'	-2.91	1.49	1.53
1	A	624	UFT	C2'-C1'	-2.91	1.49	1.53
1	A	23	UFT	C2-N3	2.91	1.43	1.38
1	A	42	UFT	C2'-C1'	-2.90	1.49	1.53
1	A	169	UFT	O4-C4	-2.90	1.18	1.24
1	A	374	UFT	C2-N3	2.90	1.43	1.38
1	A	157	CFZ	C2'-C1'	-2.90	1.49	1.53
1	A	475	UFT	O4-C4	-2.90	1.18	1.24
1	A	575	UFT	C2'-C1'	-2.90	1.49	1.53
1	A	585	UFT	O4-C4	-2.90	1.18	1.24
1	A	698	UFT	O4-C4	-2.90	1.18	1.24
1	A	303	UFT	C2-N3	2.90	1.43	1.38
1	A	283	UFT	O4-C4	-2.90	1.18	1.24
1	A	409	UFT	O4-C4	-2.90	1.18	1.24
1	A	340	UFT	C2'-C1'	-2.90	1.49	1.53
1	A	405	CFZ	C2'-C1'	-2.90	1.49	1.53
1	A	274	UFT	O4-C4	-2.89	1.18	1.24
1	A	671	UFT	O4-C4	-2.89	1.18	1.24
1	A	230	UFT	O4-C4	-2.89	1.18	1.24
1	A	521	UFT	O4-C4	-2.89	1.18	1.24
1	A	115	UFT	O4-C4	-2.89	1.18	1.24
1	A	143	UFT	O4-C4	-2.89	1.18	1.24
1	A	523	UFT	O4-C4	-2.89	1.18	1.24
1	A	589	UFT	O4-C4	-2.89	1.18	1.24
1	A	138	UFT	O4-C4	-2.89	1.18	1.24
1	A	561	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	215	UFT	O4-C4	-2.89	1.18	1.24
1	A	26	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	709	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	670	UFT	O4-C4	-2.89	1.18	1.24
1	A	597	UFT	O4-C4	-2.89	1.18	1.24
1	A	500	CFZ	O4'-C1'	2.89	1.48	1.42
1	A	705	UFT	O4-C4	-2.89	1.18	1.24
1	A	383	UFT	O4-C4	-2.89	1.18	1.24
1	A	58	UFT	O4-C4	-2.89	1.18	1.24
1	A	154	UFT	O4-C4	-2.89	1.18	1.24
1	A	378	CFZ	C2'-C1'	-2.89	1.49	1.53
1	A	555	UFT	O4-C4	-2.89	1.18	1.24
1	A	719	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	177	UFT	O4-C4	-2.88	1.18	1.24
1	A	564	CFZ	O4'-C1'	2.88	1.48	1.42
1	A	19	UFT	O4-C4	-2.88	1.18	1.24
1	A	351	UFT	O4-C4	-2.88	1.18	1.24
1	A	693	UFT	O4-C4	-2.88	1.18	1.24
1	A	685	CFZ	C2'-C1'	-2.88	1.49	1.53
1	A	350	UFT	O4-C4	-2.88	1.18	1.24
1	A	562	UFT	O4-C4	-2.88	1.18	1.24
1	A	89	UFT	O4-C4	-2.88	1.18	1.24
1	A	217	CFZ	C2'-C1'	-2.88	1.49	1.53
1	A	322	UFT	O4-C4	-2.88	1.18	1.24
1	A	116	UFT	O4-C4	-2.88	1.18	1.24
1	A	17	UFT	O4-C4	-2.87	1.18	1.24
1	A	456	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	170	UFT	O4-C4	-2.87	1.18	1.24
1	A	716	UFT	C2-N3	2.87	1.43	1.38
1	A	28	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	426	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	458	CFZ	C2'-C1'	-2.87	1.49	1.53
1	A	62	UFT	O4-C4	-2.87	1.18	1.24
1	A	345	UFT	O4-C4	-2.87	1.18	1.24
1	A	71	UFT	C2'-C1'	-2.87	1.49	1.53
1	A	194	UFT	C2-N3	2.86	1.43	1.38
1	A	71	UFT	O4-C4	-2.86	1.18	1.24
1	A	254	UFT	O4-C4	-2.86	1.18	1.24
1	A	431	UFT	O4-C4	-2.86	1.18	1.24
1	A	61	UFT	C2'-C1'	-2.86	1.49	1.53
1	A	464	UFT	C2'-C1'	-2.86	1.49	1.53
1	A	23	UFT	O4'-C1'	2.86	1.48	1.42
1	A	238	UFT	O4-C4	-2.86	1.18	1.24
1	A	504	UFT	C2-N3	2.86	1.43	1.38
1	A	311	UFT	O4-C4	-2.86	1.18	1.24
1	A	127	UFT	C2'-C1'	-2.86	1.49	1.53
1	A	234	CFZ	C2'-C1'	-2.86	1.49	1.53
1	A	601	UFT	C2'-C1'	-2.86	1.49	1.53
1	A	95	UFT	O4-C4	-2.86	1.18	1.24
1	A	672	CFZ	O4'-C1'	2.86	1.48	1.42
1	A	419	UFT	C2'-C1'	-2.86	1.49	1.53
1	A	188	UFT	O4-C4	-2.86	1.18	1.24
1	A	197	UFT	O4-C4	-2.86	1.18	1.24
1	A	588	UFT	O4-C4	-2.86	1.18	1.24
1	A	39	UFT	O4-C4	-2.85	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	662	UFT	O4-C4	-2.85	1.18	1.24
1	A	480	UFT	C2'-C1'	-2.85	1.49	1.53
1	A	573	UFT	O4-C4	-2.85	1.18	1.24
1	A	71	UFT	O4'-C1'	2.85	1.48	1.42
1	A	307	UFT	O4-C4	-2.85	1.18	1.24
1	A	451	UFT	O4-C4	-2.85	1.19	1.24
1	A	397	UFT	O4-C4	-2.85	1.19	1.24
1	A	559	UFT	C2-N3	2.85	1.42	1.38
1	A	379	CFZ	C2'-C1'	-2.84	1.49	1.53
1	A	395	CFZ	C2'-C1'	-2.84	1.49	1.53
1	A	526	CFZ	C2'-C1'	-2.84	1.49	1.53
1	A	206	CFZ	C2'-C1'	-2.84	1.49	1.53
1	A	597	UFT	C2'-C1'	-2.84	1.49	1.53
1	A	371	UFT	C2-N3	2.84	1.42	1.38
1	A	727	UFT	O4-C4	-2.84	1.19	1.24
1	A	690	CFZ	C2'-C1'	-2.84	1.49	1.53
1	A	687	UFT	C2'-C1'	-2.83	1.49	1.53
1	A	590	UFT	O4-C4	-2.83	1.19	1.24
1	A	161	CFZ	C2'-C1'	-2.83	1.49	1.53
1	A	497	UFT	O4-C4	-2.83	1.19	1.24
1	A	123	UFT	O4-C4	-2.83	1.19	1.24
1	A	686	UFT	O4-C4	-2.83	1.19	1.24
1	A	480	UFT	O4-C4	-2.83	1.19	1.24
1	A	56	UFT	C2-N3	2.83	1.42	1.38
1	A	510	UFT	O4-C4	-2.83	1.19	1.24
1	A	582	UFT	O4-C4	-2.83	1.19	1.24
1	A	724	UFT	O4-C4	-2.82	1.19	1.24
1	A	93	UFT	C2-N3	2.82	1.42	1.38
1	A	510	UFT	C2'-C1'	-2.82	1.49	1.53
1	A	485	UFT	O4-C4	-2.82	1.19	1.24
1	A	550	UFT	C2-N3	2.82	1.42	1.38
1	A	298	UFT	O4-C4	-2.82	1.19	1.24
1	A	497	UFT	O4'-C1'	2.82	1.48	1.42
1	A	655	UFT	O4-C4	-2.82	1.19	1.24
1	A	79	UFT	O4-C4	-2.81	1.19	1.24
1	A	319	UFT	O4-C4	-2.81	1.19	1.24
1	A	269	CFZ	C2'-C1'	-2.81	1.49	1.53
1	A	727	UFT	C2'-C1'	-2.81	1.49	1.53
1	A	240	UFT	O4-C4	-2.81	1.19	1.24
1	A	89	UFT	C2'-C1'	-2.81	1.49	1.53
1	A	210	UFT	C2'-C1'	-2.80	1.49	1.53
1	A	97	UFT	O4'-C1'	2.80	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	UFT	C2'-C1'	-2.80	1.49	1.53
1	A	716	UFT	O4-C4	-2.80	1.19	1.24
1	A	501	UFT	O4-C4	-2.80	1.19	1.24
1	A	713	CFZ	C2'-C1'	-2.80	1.49	1.53
1	A	151	UFT	O4-C4	-2.79	1.19	1.24
1	A	328	CFZ	C2'-C1'	-2.79	1.49	1.53
1	A	475	UFT	C2'-C1'	-2.79	1.49	1.53
1	A	175	UFT	O4'-C1'	2.78	1.48	1.42
1	A	638	UFT	C2-N3	2.78	1.42	1.38
1	A	367	UFT	O4'-C1'	2.78	1.48	1.42
1	A	107	UFT	C2'-C1'	-2.78	1.49	1.53
1	A	585	UFT	C2'-C1'	-2.78	1.49	1.53
1	A	11	CFZ	C2'-C1'	-2.78	1.49	1.53
1	A	655	UFT	C2'-C1'	-2.78	1.49	1.53
1	A	504	UFT	C2'-C1'	-2.78	1.49	1.53
1	A	51	UFT	C2-N3	2.78	1.42	1.38
1	A	374	UFT	O4'-C1'	2.77	1.48	1.42
1	A	146	CFZ	O4'-C1'	2.77	1.48	1.42
1	A	193	UFT	C2'-C1'	-2.77	1.49	1.53
1	A	94	UFT	C2-N3	2.77	1.42	1.38
1	A	361	UFT	O4'-C1'	2.77	1.48	1.42
1	A	178	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	386	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	339	UFT	C2-N3	2.77	1.42	1.38
1	A	129	CFZ	C2'-C1'	-2.77	1.49	1.53
1	A	221	UFT	O4-C4	-2.76	1.19	1.24
1	A	274	UFT	C2'-C1'	-2.76	1.49	1.53
1	A	501	UFT	C2'-C1'	-2.76	1.49	1.53
1	A	79	UFT	C2'-C1'	-2.76	1.49	1.53
1	A	210	UFT	O4'-C1'	2.76	1.48	1.42
1	A	123	UFT	C2-N3	2.76	1.42	1.38
1	A	550	UFT	C2'-C1'	-2.76	1.49	1.53
1	A	507	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	81	CFZ	C2'-C1'	-2.75	1.49	1.53
1	A	170	UFT	O4'-C1'	2.75	1.48	1.42
1	A	115	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	116	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	272	UFT	O4-C4	-2.75	1.19	1.24
1	A	33	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	432	CFZ	C2'-C1'	-2.75	1.49	1.53
1	A	360	UFT	C2-N3	2.75	1.42	1.38
1	A	562	UFT	C2'-C1'	-2.75	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	UFT	C2'-N3	2.75	1.42	1.38
1	A	254	UFT	C2'-C1'	-2.75	1.49	1.53
1	A	429	UFT	O4-C4	-2.75	1.19	1.24
1	A	95	UFT	C2'-C1'	-2.74	1.49	1.53
1	A	687	UFT	O4'-C1'	2.74	1.48	1.42
1	A	370	UFT	C2'-C1'	-2.74	1.49	1.53
1	A	663	CFZ	C2'-C1'	-2.74	1.49	1.53
1	A	601	UFT	C2-N3	2.74	1.42	1.38
1	A	356	UFT	C2-N3	2.74	1.42	1.38
1	A	192	UFT	C2'-C1'	-2.74	1.49	1.53
1	A	687	UFT	C2-N3	2.74	1.42	1.38
1	A	429	UFT	O4'-C1'	2.74	1.48	1.42
1	A	542	UFT	C2-N3	2.74	1.42	1.38
1	A	644	UFT	C2'-C1'	-2.74	1.49	1.53
1	A	154	UFT	C2'-C1'	-2.74	1.49	1.53
1	A	148	UFT	O4'-C1'	2.74	1.48	1.42
1	A	390	UFT	C2-N3	2.74	1.42	1.38
1	A	39	UFT	O4'-C1'	2.73	1.48	1.42
1	A	236	UFT	C2-N3	2.73	1.42	1.38
1	A	471	UFT	C2-N3	2.73	1.42	1.38
1	A	444	UFT	O4-C4	-2.73	1.19	1.24
1	A	727	UFT	O4'-C1'	2.73	1.48	1.42
1	A	120	UFT	C2-N3	2.73	1.42	1.38
1	A	17	UFT	O4'-C1'	2.72	1.48	1.42
1	A	693	UFT	C2'-C1'	-2.72	1.49	1.53
1	A	277	UFT	C2-N3	2.72	1.42	1.38
1	A	271	CFZ	C2'-C1'	-2.72	1.49	1.53
1	A	350	UFT	C2'-C1'	-2.72	1.49	1.53
1	A	683	UFT	C2-N3	2.72	1.42	1.38
1	A	371	UFT	O4'-C1'	2.71	1.48	1.42
1	A	559	UFT	O4'-C1'	2.71	1.48	1.42
1	A	95	UFT	C2-N3	2.71	1.42	1.38
1	A	490	CFZ	C2'-C1'	-2.71	1.49	1.53
1	A	662	UFT	C2'-C1'	-2.71	1.49	1.53
1	A	698	UFT	C2'-C1'	-2.71	1.49	1.53
1	A	686	UFT	O4'-C1'	2.70	1.48	1.42
1	A	298	UFT	O4'-C1'	2.70	1.48	1.42
1	A	171	CFZ	C2'-C1'	-2.70	1.49	1.53
1	A	388	UFT	C2'-C1'	-2.70	1.49	1.53
1	A	221	UFT	O4'-C1'	2.70	1.48	1.42
1	A	417	UFT	O4-C4	-2.70	1.19	1.24
1	A	705	UFT	C2'-C1'	-2.70	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	549	UFT	O4'-C1'	2.69	1.48	1.42
1	A	679	UFT	C2-N3	2.69	1.42	1.38
1	A	75	CFZ	C2'-C1'	-2.69	1.49	1.53
1	A	697	UFT	C2'-C1'	-2.69	1.49	1.53
1	A	374	UFT	C2'-C1'	-2.69	1.49	1.53
1	A	438	CFZ	C2'-C1'	-2.69	1.49	1.53
1	A	46	UFT	O4'-C1'	2.69	1.48	1.42
1	A	148	UFT	C2'-C1'	-2.69	1.49	1.53
1	A	578	CFZ	C2'-C1'	-2.69	1.49	1.53
1	A	590	UFT	C2'-C1'	-2.69	1.49	1.53
1	A	485	UFT	C2-N3	2.69	1.42	1.38
1	A	6	UFT	O4'-C1'	2.69	1.48	1.42
1	A	392	CFZ	C2'-C1'	-2.69	1.49	1.53
1	A	582	UFT	O4'-C1'	2.68	1.48	1.42
1	A	170	UFT	C2'-C1'	-2.68	1.49	1.53
1	A	339	UFT	O4'-C1'	2.68	1.48	1.42
1	A	697	UFT	O4'-C1'	2.68	1.48	1.42
1	A	573	UFT	O4'-C1'	2.68	1.48	1.42
1	A	46	UFT	C2'-C1'	-2.68	1.49	1.53
1	A	108	CFZ	C2'-C1'	-2.68	1.49	1.53
1	A	370	UFT	C2-N3	2.68	1.42	1.38
1	A	283	UFT	C2-N3	2.68	1.42	1.38
1	A	650	UFT	C2'-C1'	-2.68	1.49	1.53
1	A	19	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	194	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	397	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	48	UFT	O4'-C1'	2.67	1.48	1.42
1	A	346	CFZ	C2'-C1'	-2.67	1.49	1.53
1	A	409	UFT	C2-N3	2.67	1.42	1.38
1	A	56	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	238	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	181	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	44	UFT	C2-N3	2.67	1.42	1.38
1	A	33	UFT	C2-N3	2.67	1.42	1.38
1	A	612	UFT	C2-N3	2.67	1.42	1.38
1	A	476	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	559	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	558	UFT	C2-N3	2.67	1.42	1.38
1	A	523	UFT	O4'-C1'	2.67	1.48	1.42
1	A	272	UFT	O4'-C1'	2.67	1.48	1.42
1	A	451	UFT	C2'-C1'	-2.67	1.49	1.53
1	A	42	UFT	O4'-C1'	2.66	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	390	UFT	C2'-C1'	-2.66	1.49	1.53
1	A	6	UFT	C2'-C1'	-2.66	1.49	1.53
1	A	627	UFT	O4'-C1'	2.66	1.48	1.42
1	A	42	UFT	C2-N3	2.66	1.42	1.38
1	A	303	UFT	C2'-C1'	-2.66	1.49	1.53
1	A	267	UFT	C2-N3	2.66	1.42	1.38
1	A	39	UFT	C2'-C1'	-2.66	1.49	1.53
1	A	601	UFT	O4'-C1'	2.66	1.48	1.42
1	A	485	UFT	O4'-C1'	2.65	1.48	1.42
1	A	573	UFT	C2-N3	2.65	1.42	1.38
1	A	383	UFT	O4'-C1'	2.65	1.48	1.42
1	A	370	UFT	O4'-C1'	2.65	1.48	1.42
1	A	142	UFT	C2'-C1'	-2.65	1.49	1.53
1	A	39	UFT	C2-N3	2.65	1.42	1.38
1	A	556	UFT	O4'-C1'	2.65	1.48	1.42
1	A	340	UFT	O4'-C1'	2.65	1.48	1.42
1	A	340	UFT	C2-N3	2.65	1.42	1.38
1	A	66	UFT	O4'-C1'	2.65	1.48	1.42
1	A	555	UFT	O4'-C1'	2.65	1.48	1.42
1	A	197	UFT	C2'-C1'	-2.65	1.49	1.53
1	A	242	UFT	C2-N3	2.65	1.42	1.38
1	A	671	UFT	C2-N3	2.65	1.42	1.38
1	A	612	UFT	O4'-C1'	2.65	1.48	1.42
1	A	361	UFT	C2-N3	2.65	1.42	1.38
1	A	322	UFT	C2'-C1'	-2.65	1.49	1.53
1	A	607	UFT	C4-N3	2.65	1.43	1.38
1	A	213	UFT	O4'-C1'	2.65	1.48	1.42
1	A	148	UFT	C2-N3	2.65	1.42	1.38
1	A	451	UFT	O4'-C1'	2.65	1.48	1.42
1	A	549	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	638	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	683	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	62	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	120	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	267	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	638	UFT	O4'-C1'	2.64	1.48	1.42
1	A	431	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	670	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	236	UFT	O4'-C1'	2.64	1.48	1.42
1	A	532	UFT	O4-C4	-2.64	1.19	1.24
1	A	350	UFT	C2-N3	2.64	1.42	1.38
1	A	151	UFT	C2'-C1'	-2.64	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	UFT	C2-N3	2.64	1.42	1.38
1	A	167	UFT	C2-N3	2.64	1.42	1.38
1	A	595	UFT	C2-N3	2.64	1.42	1.38
1	A	175	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	617	UFT	C2'-C1'	-2.64	1.49	1.53
1	A	662	UFT	O4'-C1'	2.64	1.48	1.42
1	A	597	UFT	C2-N3	2.63	1.42	1.38
1	A	388	UFT	O4'-C1'	2.63	1.48	1.42
1	A	177	UFT	C2-N3	2.63	1.42	1.38
1	A	107	UFT	C2-N3	2.63	1.42	1.38
1	A	558	UFT	O4'-C1'	2.63	1.48	1.42
1	A	193	UFT	O4'-C1'	2.63	1.48	1.42
1	A	563	UFT	C2-N3	2.63	1.42	1.38
1	A	194	UFT	O4'-C1'	2.63	1.48	1.42
1	A	419	UFT	O4'-C1'	2.63	1.48	1.42
1	A	288	UFT	C2-N3	2.63	1.42	1.38
1	A	390	UFT	O4'-C1'	2.63	1.48	1.42
1	A	507	UFT	O4'-C1'	2.63	1.48	1.42
1	A	607	UFT	O2-C2	-2.63	1.18	1.23
1	A	138	UFT	C2-N3	2.62	1.42	1.38
1	A	288	UFT	C2'-C1'	-2.62	1.49	1.53
1	A	230	UFT	O4'-C1'	2.62	1.48	1.42
1	A	582	UFT	C2'-C1'	-2.62	1.49	1.53
1	A	254	UFT	O4'-C1'	2.62	1.48	1.42
1	A	215	UFT	C2-N3	2.62	1.42	1.38
1	A	288	UFT	O4'-C1'	2.62	1.48	1.42
1	A	429	UFT	C2-N3	2.62	1.42	1.38
1	A	311	UFT	C2-N3	2.62	1.42	1.38
1	A	107	UFT	O4'-C1'	2.62	1.48	1.42
1	A	421	UFT	O4'-C1'	2.62	1.48	1.42
1	A	360	UFT	O4'-C1'	2.62	1.48	1.42
1	A	89	UFT	C2-N3	2.62	1.42	1.38
1	A	642	UFT	C2'-C1'	-2.61	1.49	1.53
1	A	521	UFT	C2-N3	2.61	1.42	1.38
1	A	197	UFT	C2-N3	2.61	1.42	1.38
1	A	388	UFT	C2-N3	2.61	1.42	1.38
1	A	556	UFT	C2-N3	2.61	1.42	1.38
1	A	397	UFT	C2-N3	2.61	1.42	1.38
1	A	33	UFT	O4'-C1'	2.61	1.48	1.42
1	A	6	UFT	C2-N3	2.61	1.42	1.38
1	A	644	UFT	C2-N3	2.61	1.42	1.38
1	A	240	UFT	C2'-C1'	-2.61	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	UFT	C2-N3	2.61	1.42	1.38
1	A	196	UFT	C2-N3	2.61	1.42	1.38
1	A	597	UFT	O4'-C1'	2.61	1.48	1.42
1	A	464	UFT	C2-N3	2.60	1.42	1.38
1	A	650	UFT	O4'-C1'	2.60	1.48	1.42
1	A	19	UFT	O4'-C1'	2.60	1.48	1.42
1	A	56	UFT	O4'-C1'	2.60	1.48	1.42
1	A	727	UFT	C2-N3	2.60	1.42	1.38
1	A	97	UFT	C2-N3	2.60	1.42	1.38
1	A	507	UFT	C2-N3	2.60	1.42	1.38
1	A	504	UFT	O4'-C1'	2.60	1.48	1.42
1	A	475	UFT	C2-N3	2.60	1.42	1.38
1	A	643	UFT	O4'-C1'	2.60	1.48	1.42
1	A	17	UFT	C2-N3	2.60	1.42	1.38
1	A	421	UFT	C2-N3	2.60	1.42	1.38
1	A	93	UFT	O4'-C1'	2.60	1.48	1.42
1	A	642	UFT	O4'-C1'	2.60	1.48	1.42
1	A	417	UFT	O4'-C1'	2.60	1.48	1.42
1	A	62	UFT	C2-N3	2.60	1.42	1.38
1	A	93	UFT	C2'-C1'	-2.60	1.50	1.53
1	A	319	UFT	C2'-C1'	-2.60	1.50	1.53
1	A	175	UFT	C2-N3	2.60	1.42	1.38
1	A	48	UFT	C2'-C1'	-2.59	1.50	1.53
1	A	705	UFT	C2-N3	2.59	1.42	1.38
1	A	329	UFT	O4'-C1'	2.59	1.48	1.42
1	A	193	UFT	C2-N3	2.59	1.42	1.38
1	A	555	UFT	C2'-C1'	-2.59	1.50	1.53
1	A	192	UFT	O4'-C1'	2.59	1.48	1.42
1	A	116	UFT	C2-N3	2.59	1.42	1.38
1	A	471	UFT	O4'-C1'	2.59	1.48	1.42
1	A	19	UFT	C2-N3	2.59	1.42	1.38
1	A	142	UFT	C2-N3	2.59	1.42	1.38
1	A	662	UFT	C2-N3	2.59	1.42	1.38
1	A	542	UFT	O4'-C1'	2.59	1.48	1.42
1	A	322	UFT	O4'-C1'	2.59	1.48	1.42
1	A	94	UFT	C2'-C1'	-2.59	1.50	1.53
1	A	277	UFT	C2'-C1'	-2.59	1.50	1.53
1	A	151	UFT	O4'-C1'	2.58	1.48	1.42
1	A	595	UFT	C2'-C1'	-2.58	1.50	1.53
1	A	94	UFT	O4'-C1'	2.58	1.48	1.42
1	A	698	UFT	C2-N3	2.58	1.42	1.38
1	A	274	UFT	C2-N3	2.58	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	693	UFT	C2-N3	2.58	1.42	1.38
1	A	116	UFT	O4'-C1'	2.58	1.48	1.42
1	A	170	UFT	C2-N3	2.58	1.42	1.38
1	A	431	UFT	C2-N3	2.58	1.42	1.38
1	A	444	UFT	C2'-C1'	-2.58	1.50	1.53
1	A	240	UFT	C2-N3	2.58	1.42	1.38
1	A	686	UFT	C2-N3	2.58	1.42	1.38
1	A	215	UFT	O4'-C1'	2.57	1.48	1.42
1	A	254	UFT	C2-N3	2.57	1.42	1.38
1	A	549	UFT	C2-N3	2.57	1.42	1.38
1	A	350	UFT	O4'-C1'	2.57	1.47	1.42
1	A	697	UFT	C2-N3	2.57	1.42	1.38
1	A	409	UFT	O4'-C1'	2.57	1.47	1.42
1	A	351	UFT	C2'-C1'	-2.57	1.50	1.53
1	A	371	UFT	C2'-C1'	-2.57	1.50	1.53
1	A	267	UFT	O4'-C1'	2.57	1.47	1.42
1	A	154	UFT	C2-N3	2.57	1.42	1.38
1	A	48	UFT	C2-N3	2.57	1.42	1.38
1	A	215	UFT	C2'-C1'	-2.57	1.50	1.53
1	A	644	UFT	O4'-C1'	2.57	1.47	1.42
1	A	95	UFT	O4'-C1'	2.57	1.47	1.42
1	A	127	UFT	O4'-C1'	2.57	1.47	1.42
1	A	377	UFT	C2-N3	2.57	1.42	1.38
1	A	79	UFT	O4'-C1'	2.57	1.47	1.42
1	A	138	UFT	O4'-C1'	2.57	1.47	1.42
1	A	521	UFT	O4'-C1'	2.57	1.47	1.42
1	A	169	UFT	C2-N3	2.57	1.42	1.38
1	A	562	UFT	C2-N3	2.57	1.42	1.38
1	A	550	UFT	O4'-C1'	2.57	1.47	1.42
1	A	79	UFT	C2-N3	2.57	1.42	1.38
1	A	670	UFT	C2-N3	2.56	1.42	1.38
1	A	58	UFT	C2-N3	2.56	1.42	1.38
1	A	588	UFT	C2-N3	2.56	1.42	1.38
1	A	471	UFT	C4-N3	2.56	1.43	1.38
1	A	88	UFT	C2-N3	2.56	1.42	1.38
1	A	501	UFT	O4'-C1'	2.56	1.47	1.42
1	A	23	UFT	C2'-C1'	-2.56	1.50	1.53
1	A	230	UFT	C2-N3	2.56	1.42	1.38
1	A	616	UFT	C2'-C1'	-2.56	1.50	1.53
1	A	419	UFT	C2-N3	2.56	1.42	1.38
1	A	167	UFT	C2'-C1'	-2.56	1.50	1.53
1	A	444	UFT	O4'-C1'	2.56	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	624	UFT	O4'-C1'	2.56	1.47	1.42
1	A	143	UFT	C2-N3	2.56	1.42	1.38
1	A	307	UFT	C2-N3	2.56	1.42	1.38
1	A	319	UFT	C2-N3	2.55	1.42	1.38
1	A	143	UFT	C2'-C1'	-2.55	1.50	1.53
1	A	188	UFT	O4'-C1'	2.55	1.47	1.42
1	A	263	UFT	C2'-C1'	-2.55	1.50	1.53
1	A	617	UFT	C2-N3	2.55	1.42	1.38
1	A	356	UFT	C2'-C1'	-2.55	1.50	1.53
1	A	61	UFT	C2-N3	2.55	1.42	1.38
1	A	555	UFT	C2-N3	2.55	1.42	1.38
1	A	115	UFT	C2-N3	2.55	1.42	1.38
1	A	123	UFT	O4'-C1'	2.55	1.47	1.42
1	A	705	UFT	O4'-C1'	2.55	1.47	1.42
1	A	464	UFT	O4'-C1'	2.55	1.47	1.42
1	A	643	UFT	C2-N3	2.55	1.42	1.38
1	A	693	UFT	O4'-C1'	2.55	1.47	1.42
1	A	242	UFT	C2'-C1'	-2.55	1.50	1.53
1	A	377	UFT	O2-C2	-2.55	1.18	1.23
1	A	617	UFT	O4'-C1'	2.54	1.47	1.42
1	A	127	UFT	C2-N3	2.54	1.42	1.38
1	A	616	UFT	O4'-C1'	2.54	1.47	1.42
1	A	655	UFT	C2-N3	2.54	1.42	1.38
1	A	671	UFT	C2'-C1'	-2.54	1.50	1.53
1	A	32	UFT	O4'-C1'	2.54	1.47	1.42
1	A	274	UFT	O4'-C1'	2.54	1.47	1.42
1	A	476	UFT	O4'-C1'	2.54	1.47	1.42
1	A	670	UFT	O4'-C1'	2.54	1.47	1.42
1	A	532	UFT	C2'-C1'	-2.54	1.50	1.53
1	A	463	CFZ	C2'-C1'	-2.54	1.50	1.53
1	A	451	UFT	C2-N3	2.54	1.42	1.38
1	A	476	UFT	C2-N3	2.54	1.42	1.38
1	A	590	UFT	C2-N3	2.54	1.42	1.38
1	A	143	UFT	O4'-C1'	2.54	1.47	1.42
1	A	263	UFT	O4'-C1'	2.54	1.47	1.42
1	A	197	UFT	O4'-C1'	2.54	1.47	1.42
1	A	431	UFT	O4'-C1'	2.54	1.47	1.42
1	A	322	UFT	C2-N3	2.53	1.42	1.38
1	A	356	UFT	O4'-C1'	2.53	1.47	1.42
1	A	563	UFT	O4'-C1'	2.53	1.47	1.42
1	A	667	UFT	C2-N3	2.53	1.42	1.38
1	A	383	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	501	UFT	C2-N3	2.53	1.42	1.38
1	A	667	UFT	O4'-C1'	2.53	1.47	1.42
1	A	238	UFT	O4'-C1'	2.53	1.47	1.42
1	A	616	UFT	C2-N3	2.53	1.42	1.38
1	A	319	UFT	O4'-C1'	2.53	1.47	1.42
1	A	575	UFT	C2-N3	2.53	1.42	1.38
1	A	167	UFT	O4'-C1'	2.53	1.47	1.42
1	A	624	UFT	C2-N3	2.52	1.42	1.38
1	A	131	CFZ	C2'-C1'	-2.52	1.50	1.53
1	A	377	UFT	C2'-C1'	-2.52	1.50	1.53
1	A	627	UFT	C2-N3	2.52	1.42	1.38
1	A	61	UFT	O4'-C1'	2.52	1.47	1.42
1	A	397	UFT	O4'-C1'	2.52	1.47	1.42
1	A	196	UFT	C2'-C1'	-2.52	1.50	1.53
1	A	192	UFT	C2-N3	2.52	1.42	1.38
1	A	283	UFT	O4'-C1'	2.52	1.47	1.42
1	A	89	UFT	O4'-C1'	2.52	1.47	1.42
1	A	32	UFT	C2-N3	2.52	1.42	1.38
1	A	272	UFT	C2-N3	2.52	1.42	1.38
1	A	44	UFT	O4'-C1'	2.52	1.47	1.42
1	A	377	UFT	O4'-C1'	2.52	1.47	1.42
1	A	115	UFT	O4'-C1'	2.52	1.47	1.42
1	A	151	UFT	C2-N3	2.52	1.42	1.38
1	A	351	UFT	O4'-C1'	2.51	1.47	1.42
1	A	585	UFT	O4'-C1'	2.51	1.47	1.42
1	A	221	UFT	C2-N3	2.51	1.42	1.38
1	A	487	CFZ	C2'-C1'	-2.51	1.50	1.53
1	A	238	UFT	C2-N3	2.51	1.42	1.38
1	A	575	UFT	O4'-C1'	2.51	1.47	1.42
1	A	230	UFT	C2'-C1'	-2.51	1.50	1.53
1	A	589	UFT	C2-N3	2.51	1.42	1.38
1	A	169	UFT	O4'-C1'	2.50	1.47	1.42
1	A	421	UFT	C2'-C1'	-2.50	1.50	1.53
1	A	655	UFT	O4'-C1'	2.50	1.47	1.42
1	A	468	UFT	C2-N3	2.50	1.42	1.38
1	A	607	UFT	O4'-C1'	2.50	1.47	1.42
1	A	719	UFT	C2-N3	2.50	1.42	1.38
1	A	188	UFT	C2-N3	2.50	1.42	1.38
1	A	88	UFT	O4'-C1'	2.50	1.47	1.42
1	A	138	UFT	C2'-C1'	-2.50	1.50	1.53
1	A	679	UFT	C2'-C1'	-2.49	1.50	1.53
1	A	307	UFT	O4'-C1'	2.49	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	UFT	O4'-C1'	2.49	1.47	1.42
1	A	240	UFT	O4'-C1'	2.49	1.47	1.42
1	A	671	UFT	O4'-C1'	2.49	1.47	1.42
1	A	17	UFT	C2'-C1'	-2.49	1.50	1.53
1	A	607	UFT	C2-N3	2.49	1.42	1.38
1	A	585	UFT	C2-N3	2.49	1.42	1.38
1	A	345	UFT	C2-N3	2.49	1.42	1.38
1	A	88	UFT	C2'-C1'	-2.48	1.50	1.53
1	A	497	UFT	C2-N3	2.48	1.42	1.38
1	A	627	UFT	C2'-C1'	-2.48	1.50	1.53
1	A	523	UFT	C2-N3	2.48	1.42	1.38
1	A	588	UFT	O2-C2	-2.48	1.18	1.23
1	A	351	UFT	C2-N3	2.48	1.42	1.38
1	A	58	UFT	O2-C2	-2.48	1.18	1.23
1	A	32	UFT	C2'-C1'	-2.48	1.50	1.53
1	A	562	UFT	O4'-C1'	2.47	1.47	1.42
1	A	242	UFT	O4'-C1'	2.47	1.47	1.42
1	A	679	UFT	O4'-C1'	2.47	1.47	1.42
1	A	542	UFT	C2'-C1'	-2.47	1.50	1.53
1	A	429	UFT	C2'-C1'	-2.47	1.50	1.53
1	A	719	UFT	C2'-C1'	-2.47	1.50	1.53
1	A	444	UFT	C2-N3	2.47	1.42	1.38
1	A	329	UFT	C2-N3	2.47	1.42	1.38
1	A	588	UFT	C2'-C1'	-2.46	1.50	1.53
1	A	303	UFT	O4'-C1'	2.46	1.47	1.42
1	A	686	UFT	C2'-C1'	-2.46	1.50	1.53
1	A	724	UFT	O4'-C1'	2.46	1.47	1.42
1	A	169	UFT	C2'-C1'	-2.46	1.50	1.53
1	A	589	UFT	C2'-C1'	-2.46	1.50	1.53
1	A	621	CFZ	C2'-C1'	-2.46	1.50	1.53
1	A	409	UFT	C2'-C1'	-2.46	1.50	1.53
1	A	724	UFT	C2-N3	2.45	1.42	1.38
1	A	277	UFT	O4'-C1'	2.45	1.47	1.42
1	A	683	UFT	O4'-C1'	2.45	1.47	1.42
1	A	589	UFT	O4'-C1'	2.45	1.47	1.42
1	A	563	UFT	C2'-C1'	-2.44	1.50	1.53
1	A	123	UFT	C2'-C1'	-2.44	1.50	1.53
1	A	698	UFT	O4'-C1'	2.44	1.47	1.42
1	A	360	UFT	C2'-C1'	-2.44	1.50	1.53
1	A	468	UFT	O2-C2	-2.44	1.18	1.23
1	A	58	UFT	O4'-C1'	2.44	1.47	1.42
1	A	272	UFT	C2'-C1'	-2.44	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	UFT	C2'-C1'	-2.44	1.50	1.53
1	A	115	UFT	O2-C2	-2.43	1.18	1.23
1	A	642	UFT	C2-N3	2.43	1.42	1.38
1	A	417	UFT	C2-N3	2.43	1.42	1.38
1	A	62	UFT	O4'-C1'	2.43	1.47	1.42
1	A	475	UFT	O4'-C1'	2.43	1.47	1.42
1	A	523	UFT	C2'-C1'	-2.43	1.50	1.53
1	A	480	UFT	O4'-C1'	2.43	1.47	1.42
1	A	51	UFT	O4'-C1'	2.43	1.47	1.42
1	A	196	UFT	O4'-C1'	2.43	1.47	1.42
1	A	716	UFT	O4'-C1'	2.42	1.47	1.42
1	A	590	UFT	O4'-C1'	2.42	1.47	1.42
1	A	177	UFT	O4'-C1'	2.42	1.47	1.42
1	A	177	UFT	C2'-C1'	-2.42	1.50	1.53
1	A	181	UFT	O4-C4	-2.41	1.19	1.24
1	A	188	UFT	C2'-C1'	-2.41	1.50	1.53
1	A	361	UFT	O2-C2	-2.41	1.18	1.23
1	A	532	UFT	O4'-C1'	2.41	1.47	1.42
1	A	154	UFT	O2-C2	-2.41	1.18	1.23
1	A	120	UFT	O4'-C1'	2.41	1.47	1.42
1	A	719	UFT	O4'-C1'	2.40	1.47	1.42
1	A	556	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	307	UFT	C2'-C1'	-2.40	1.50	1.53
1	A	319	UFT	O2-C2	-2.40	1.18	1.23
1	A	601	UFT	O2-C2	-2.40	1.18	1.23
1	A	127	UFT	O2-C2	-2.40	1.18	1.23
1	A	595	UFT	O4'-C1'	2.39	1.47	1.42
1	A	167	UFT	O2-C2	-2.39	1.18	1.23
1	A	417	UFT	C2'-C1'	-2.39	1.50	1.53
1	A	298	UFT	C2-N3	2.39	1.42	1.38
1	A	123	UFT	O2-C2	-2.38	1.18	1.23
1	A	194	UFT	C4-N3	2.38	1.42	1.38
1	A	181	UFT	O4'-C1'	2.38	1.47	1.42
1	A	476	UFT	O2-C2	-2.38	1.18	1.23
1	A	421	UFT	O2-C2	-2.38	1.18	1.23
1	A	468	UFT	O4'-C1'	2.38	1.47	1.42
1	A	601	UFT	C4-N3	2.38	1.42	1.38
1	A	51	UFT	O2-C2	-2.38	1.18	1.23
1	A	510	UFT	O4'-C1'	2.38	1.47	1.42
1	A	582	UFT	O2-C2	-2.38	1.18	1.23
1	A	242	UFT	O2-C2	-2.37	1.18	1.23
1	A	510	UFT	C2-N3	2.37	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	693	UFT	O2-C2	-2.37	1.18	1.23
1	A	345	UFT	O4'-C1'	2.37	1.47	1.42
1	A	563	UFT	O2-C2	-2.37	1.18	1.23
1	A	95	UFT	O2-C2	-2.37	1.18	1.23
1	A	612	UFT	O2-C2	-2.37	1.18	1.23
1	A	79	UFT	O2-C2	-2.37	1.18	1.23
1	A	329	UFT	O2-C2	-2.36	1.18	1.23
1	A	562	UFT	O2-C2	-2.36	1.18	1.23
1	A	283	UFT	C4-N3	2.36	1.42	1.38
1	A	213	UFT	O2-C2	-2.36	1.18	1.23
1	A	687	UFT	O2-C2	-2.36	1.18	1.23
1	A	383	UFT	O2-C2	-2.36	1.18	1.23
1	A	480	UFT	C2-N3	2.36	1.42	1.38
1	A	193	UFT	O2-C2	-2.36	1.18	1.23
1	A	272	UFT	O2-C2	-2.36	1.18	1.23
1	A	62	UFT	O2-C2	-2.36	1.18	1.23
1	A	575	UFT	O2-C2	-2.36	1.18	1.23
1	A	339	UFT	C2'-C1'	-2.36	1.50	1.53
1	A	510	UFT	O2-C2	-2.35	1.18	1.23
1	A	17	UFT	O2-C2	-2.35	1.18	1.23
1	A	638	UFT	C4-N3	2.35	1.42	1.38
1	A	42	UFT	O2-C2	-2.35	1.18	1.23
1	A	56	UFT	C4-N3	2.35	1.42	1.38
1	A	642	UFT	O2-C2	-2.35	1.18	1.23
1	A	662	UFT	O2-C2	-2.35	1.18	1.23
1	A	559	UFT	O2-C2	-2.35	1.18	1.23
1	A	624	UFT	O2-C2	-2.35	1.18	1.23
1	A	32	UFT	O2-C2	-2.35	1.18	1.23
1	A	238	UFT	O2-C2	-2.35	1.18	1.23
1	A	56	UFT	O2-C2	-2.34	1.18	1.23
1	A	644	UFT	O2-C2	-2.34	1.18	1.23
1	A	444	UFT	O2-C2	-2.34	1.18	1.23
1	A	686	UFT	O2-C2	-2.34	1.18	1.23
1	A	724	UFT	O2-C2	-2.34	1.18	1.23
1	A	697	UFT	O2-C2	-2.34	1.18	1.23
1	A	573	UFT	C2'-C1'	-2.34	1.50	1.53
1	A	61	UFT	O2-C2	-2.34	1.18	1.23
1	A	181	UFT	O2-C2	-2.34	1.18	1.23
1	A	367	UFT	O2-C2	-2.34	1.18	1.23
1	A	670	UFT	O2-C2	-2.34	1.18	1.23
1	A	151	UFT	O2-C2	-2.34	1.18	1.23
1	A	170	UFT	O2-C2	-2.34	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	UFT	O2-C2	-2.34	1.18	1.23
1	A	698	UFT	O2-C2	-2.34	1.18	1.23
1	A	655	UFT	O2-C2	-2.34	1.18	1.23
1	A	431	UFT	O2-C2	-2.34	1.18	1.23
1	A	197	UFT	O2-C2	-2.33	1.18	1.23
1	A	142	UFT	O2-C2	-2.33	1.18	1.23
1	A	33	UFT	O2-C2	-2.33	1.18	1.23
1	A	311	UFT	O4'-C1'	2.33	1.47	1.42
1	A	263	UFT	O2-C2	-2.33	1.18	1.23
1	A	638	UFT	O2-C2	-2.33	1.18	1.23
1	A	397	UFT	O2-C2	-2.33	1.18	1.23
1	A	671	UFT	O2-C2	-2.33	1.18	1.23
1	A	582	UFT	C2-N3	2.33	1.42	1.38
1	A	88	UFT	O2-C2	-2.33	1.18	1.23
1	A	303	UFT	C4-N3	2.33	1.42	1.38
1	A	501	UFT	O2-C2	-2.33	1.18	1.23
1	A	367	UFT	C2'-C1'	-2.33	1.50	1.53
1	A	573	UFT	O2-C2	-2.33	1.18	1.23
1	A	44	UFT	O2-C2	-2.33	1.18	1.23
1	A	236	UFT	O2-C2	-2.32	1.18	1.23
1	A	521	UFT	O2-C2	-2.32	1.18	1.23
1	A	138	UFT	O2-C2	-2.32	1.18	1.23
1	A	356	UFT	O2-C2	-2.32	1.18	1.23
1	A	409	UFT	O2-C2	-2.32	1.18	1.23
1	A	468	UFT	C2'-C1'	-2.32	1.50	1.53
1	A	374	UFT	O2-C2	-2.32	1.19	1.23
1	A	360	UFT	O2-C2	-2.32	1.19	1.23
1	A	471	UFT	O2-C2	-2.32	1.19	1.23
1	A	532	UFT	O2-C2	-2.32	1.19	1.23
1	A	595	UFT	O2-C2	-2.31	1.19	1.23
1	A	559	UFT	C4-N3	2.31	1.42	1.38
1	A	94	UFT	O2-C2	-2.31	1.19	1.23
1	A	485	UFT	O2-C2	-2.31	1.19	1.23
1	A	194	UFT	O2-C2	-2.31	1.19	1.23
1	A	339	UFT	O2-C2	-2.31	1.19	1.23
1	A	89	UFT	O2-C2	-2.31	1.19	1.23
1	A	643	UFT	O2-C2	-2.31	1.19	1.23
1	A	340	UFT	O2-C2	-2.31	1.19	1.23
1	A	532	UFT	C2-N3	2.31	1.42	1.38
1	A	142	UFT	O4'-C1'	2.31	1.47	1.42
1	A	23	UFT	O2-C2	-2.31	1.19	1.23
1	A	322	UFT	O2-C2	-2.31	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	550	UFT	O2-C2	-2.31	1.19	1.23
1	A	542	UFT	O2-C2	-2.30	1.19	1.23
1	A	585	UFT	O2-C2	-2.30	1.19	1.23
1	A	679	UFT	O2-C2	-2.30	1.19	1.23
1	A	643	UFT	C2'-C1'	-2.30	1.50	1.53
1	A	210	UFT	O2-C2	-2.30	1.19	1.23
1	A	283	UFT	O2-C2	-2.30	1.19	1.23
1	A	283	UFT	C2'-C1'	-2.30	1.50	1.53
1	A	370	UFT	O2-C2	-2.29	1.19	1.23
1	A	254	UFT	O2-C2	-2.29	1.19	1.23
1	A	716	UFT	C4-N3	2.29	1.42	1.38
1	A	371	UFT	O2-C2	-2.29	1.19	1.23
1	A	589	UFT	O2-C2	-2.29	1.19	1.23
1	A	196	UFT	O2-C2	-2.29	1.19	1.23
1	A	303	UFT	O2-C2	-2.29	1.19	1.23
1	A	597	UFT	O2-C2	-2.29	1.19	1.23
1	A	277	UFT	C4-N3	2.29	1.42	1.38
1	A	616	UFT	O2-C2	-2.29	1.19	1.23
1	A	460	CFZ	C6-C5	2.29	1.40	1.35
1	A	674	CFZ	C6-C5	2.29	1.40	1.35
1	A	307	UFT	O2-C2	-2.29	1.19	1.23
1	A	143	UFT	O2-C2	-2.29	1.19	1.23
1	A	93	UFT	O2-C2	-2.28	1.19	1.23
1	A	480	UFT	O2-C2	-2.28	1.19	1.23
1	A	390	UFT	O2-C2	-2.28	1.19	1.23
1	A	19	UFT	O2-C2	-2.28	1.19	1.23
1	A	683	UFT	O2-C2	-2.28	1.19	1.23
1	A	192	UFT	O2-C2	-2.28	1.19	1.23
1	A	617	UFT	O2-C2	-2.28	1.19	1.23
1	A	116	UFT	O2-C2	-2.28	1.19	1.23
1	A	417	UFT	O2-C2	-2.28	1.19	1.23
1	A	267	UFT	O2-C2	-2.28	1.19	1.23
1	A	351	UFT	O2-C2	-2.28	1.19	1.23
1	A	590	UFT	O2-C2	-2.28	1.19	1.23
1	A	558	UFT	O2-C2	-2.28	1.19	1.23
1	A	667	UFT	O2-C2	-2.28	1.19	1.23
1	A	288	UFT	O2-C2	-2.28	1.19	1.23
1	A	719	UFT	O2-C2	-2.27	1.19	1.23
1	A	107	UFT	O2-C2	-2.27	1.19	1.23
1	A	588	UFT	O4'-C1'	2.27	1.47	1.42
1	A	550	UFT	C4-N3	2.27	1.42	1.38
1	A	274	UFT	O2-C2	-2.27	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	555	UFT	O2-C2	-2.27	1.19	1.23
1	A	504	UFT	O2-C2	-2.27	1.19	1.23
1	A	240	UFT	O2-C2	-2.27	1.19	1.23
1	A	215	UFT	O2-C2	-2.26	1.19	1.23
1	A	221	UFT	O2-C2	-2.26	1.19	1.23
1	A	66	UFT	O2-C2	-2.26	1.19	1.23
1	A	169	UFT	O2-C2	-2.26	1.19	1.23
1	A	311	UFT	O2-C2	-2.26	1.19	1.23
1	A	507	UFT	O2-C2	-2.26	1.19	1.23
1	A	371	UFT	C4-N3	2.26	1.42	1.38
1	A	464	UFT	O2-C2	-2.26	1.19	1.23
1	A	65	CFZ	C6-C5	2.26	1.40	1.35
1	A	120	UFT	O2-C2	-2.25	1.19	1.23
1	A	595	UFT	C4-N3	2.25	1.42	1.38
1	A	230	UFT	O2-C2	-2.25	1.19	1.23
1	A	716	UFT	C2'-C1'	-2.25	1.50	1.53
1	A	386	CFZ	C6-C5	2.25	1.40	1.35
1	A	48	UFT	O2-C2	-2.25	1.19	1.23
1	A	6	UFT	O2-C2	-2.25	1.19	1.23
1	A	188	UFT	O2-C2	-2.25	1.19	1.23
1	A	705	UFT	O2-C2	-2.25	1.19	1.23
1	A	97	UFT	O2-C2	-2.25	1.19	1.23
1	A	277	UFT	O2-C2	-2.24	1.19	1.23
1	A	556	UFT	O2-C2	-2.24	1.19	1.23
1	A	236	UFT	C4-N3	2.24	1.42	1.38
1	A	451	UFT	O2-C2	-2.24	1.19	1.23
1	A	687	UFT	C4-N3	2.24	1.42	1.38
1	A	497	UFT	O2-C2	-2.24	1.19	1.23
1	A	523	UFT	O2-C2	-2.24	1.19	1.23
1	A	144	CFZ	C6-C5	2.24	1.40	1.35
1	A	177	UFT	O2-C2	-2.24	1.19	1.23
1	A	502	CFZ	C6-C5	2.23	1.40	1.35
1	A	538	CFZ	C6-C5	2.23	1.40	1.35
1	A	578	CFZ	C6-C5	2.23	1.40	1.35
1	A	727	UFT	O2-C2	-2.23	1.19	1.23
1	A	650	UFT	C4-N3	2.23	1.42	1.38
1	A	298	UFT	O2-C2	-2.22	1.19	1.23
1	A	298	UFT	C2'-C1'	-2.22	1.50	1.53
1	A	350	UFT	O2-C2	-2.22	1.19	1.23
1	A	175	UFT	O2-C2	-2.22	1.19	1.23
1	A	497	UFT	C2'-C1'	-2.22	1.50	1.53
1	A	650	UFT	O2-C2	-2.21	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	UFT	O2-C2	-2.21	1.19	1.23
1	A	55	CFZ	C6-C5	2.21	1.40	1.35
1	A	558	UFT	C4-N3	2.21	1.42	1.38
1	A	429	UFT	O2-C2	-2.21	1.19	1.23
1	A	148	UFT	O2-C2	-2.21	1.19	1.23
1	A	367	UFT	C4-N3	2.20	1.42	1.38
1	A	120	UFT	C4-N3	2.20	1.42	1.38
1	A	210	UFT	C4-N3	2.20	1.42	1.38
1	A	405	CFZ	C6-C5	2.19	1.40	1.35
1	A	117	CFZ	C6-C5	2.19	1.40	1.35
1	A	426	CFZ	C6-C5	2.19	1.40	1.35
1	A	46	UFT	O2-C2	-2.19	1.19	1.23
1	A	171	CFZ	C6-C5	2.19	1.40	1.35
1	A	263	UFT	C4-N3	2.19	1.42	1.38
1	A	114	CFZ	C6-C5	2.18	1.40	1.35
1	A	490	CFZ	C6-C5	2.18	1.40	1.35
1	A	699	CFZ	C6-C5	2.18	1.40	1.35
1	A	627	UFT	O2-C2	-2.18	1.19	1.23
1	A	419	UFT	O2-C2	-2.18	1.19	1.23
1	A	93	UFT	C4-N3	2.18	1.42	1.38
1	A	181	UFT	C2-N3	2.17	1.41	1.38
1	A	661	CFZ	C6-C5	2.17	1.40	1.35
1	A	728	CFZ	C6-C5	2.17	1.40	1.35
1	A	656	CFZ	C6-C5	2.17	1.40	1.35
1	A	663	CFZ	C6-C5	2.17	1.40	1.35
1	A	107	UFT	C4-N3	2.17	1.42	1.38
1	A	80	CFZ	C6-C5	2.16	1.40	1.35
1	A	90	CFZ	C6-C5	2.16	1.40	1.35
1	A	618	CFZ	C6-C5	2.16	1.40	1.35
1	A	233	CFZ	C6-C5	2.16	1.40	1.35
1	A	409	UFT	C4-N3	2.16	1.42	1.38
1	A	645	CFZ	C6-C5	2.15	1.40	1.35
1	A	123	UFT	C4-N3	2.15	1.42	1.38
1	A	388	UFT	O2-C2	-2.15	1.19	1.23
1	A	716	UFT	O2-C2	-2.15	1.19	1.23
1	A	621	CFZ	C6-C5	2.15	1.40	1.35
1	A	51	UFT	C4-N3	2.15	1.42	1.38
1	A	542	UFT	C4-N3	2.15	1.42	1.38
1	A	653	CFZ	C6-C5	2.15	1.40	1.35
1	A	81	CFZ	C6-C5	2.15	1.40	1.35
1	A	198	CFZ	C6-C5	2.15	1.40	1.35
1	A	602	CFZ	C6-C5	2.15	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	CFZ	C6-C5	2.14	1.40	1.35
1	A	33	UFT	C4-N3	2.14	1.42	1.38
1	A	631	CFZ	C6-C5	2.14	1.40	1.35
1	A	693	UFT	C4-N3	2.14	1.42	1.38
1	A	302	CFZ	C6-C5	2.14	1.40	1.35
1	A	672	CFZ	C6-C5	2.14	1.40	1.35
1	A	605	CFZ	C6-C5	2.13	1.40	1.35
1	A	356	UFT	C4-N3	2.13	1.42	1.38
1	A	128	CFZ	C6-C5	2.13	1.40	1.35
1	A	456	CFZ	C6-C5	2.13	1.40	1.35
1	A	15	CFZ	C6-C5	2.13	1.40	1.35
1	A	561	CFZ	C6-C5	2.13	1.40	1.35
1	A	392	CFZ	C6-C5	2.13	1.40	1.35
1	A	395	CFZ	C6-C5	2.13	1.40	1.35
1	A	291	CFZ	C6-C5	2.13	1.40	1.35
1	A	6	UFT	C4-N3	2.13	1.42	1.38
1	A	89	UFT	C4-N3	2.13	1.42	1.38
1	A	603	CFZ	C6-C5	2.13	1.40	1.35
1	A	564	CFZ	C6-C5	2.12	1.40	1.35
1	A	574	CFZ	C6-C5	2.12	1.40	1.35
1	A	487	CFZ	C6-C5	2.12	1.40	1.35
1	A	155	CFZ	C6-C5	2.12	1.40	1.35
1	A	591	CFZ	C6-C5	2.12	1.40	1.35
1	A	679	UFT	C4-N3	2.12	1.42	1.38
1	A	362	CFZ	C6-C5	2.12	1.40	1.35
1	A	458	CFZ	C6-C5	2.12	1.40	1.35
1	A	604	CFZ	C6-C5	2.12	1.40	1.35
1	A	536	CFZ	C6-C5	2.12	1.40	1.35
1	A	26	CFZ	C6-C5	2.12	1.40	1.35
1	A	637	CFZ	C6-C5	2.12	1.40	1.35
1	A	230	UFT	C4-N3	2.12	1.42	1.38
1	A	464	UFT	C4-N3	2.12	1.42	1.38
1	A	629	CFZ	C6-C5	2.12	1.40	1.35
1	A	328	CFZ	C6-C5	2.12	1.40	1.35
1	A	483	CFZ	C6-C5	2.12	1.40	1.35
1	A	549	UFT	O2-C2	-2.11	1.19	1.23
1	A	635	CFZ	C6-C5	2.11	1.40	1.35
1	A	467	CFZ	C6-C5	2.11	1.40	1.35
1	A	473	CFZ	C6-C5	2.11	1.40	1.35
1	A	594	CFZ	C6-C5	2.11	1.40	1.35
1	A	720	CFZ	C6-C5	2.11	1.40	1.35
1	A	346	CFZ	C6-C5	2.11	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	UFT	O2-C2	-2.11	1.19	1.23
1	A	161	CFZ	C6-C5	2.11	1.40	1.35
1	A	234	CFZ	C6-C5	2.11	1.40	1.35
1	A	366	CFZ	C6-C5	2.11	1.40	1.35
1	A	58	UFT	C4-N3	2.11	1.42	1.38
1	A	193	UFT	C4-N3	2.11	1.42	1.38
1	A	242	UFT	C4-N3	2.11	1.42	1.38
1	A	689	CFZ	C6-C5	2.11	1.40	1.35
1	A	244	CFZ	C6-C5	2.10	1.40	1.35
1	A	390	UFT	C4-N3	2.10	1.42	1.38
1	A	624	UFT	C4-N3	2.10	1.42	1.38
1	A	644	UFT	C4-N3	2.10	1.42	1.38
1	A	407	CFZ	C6-C5	2.10	1.40	1.35
1	A	657	CFZ	C6-C5	2.10	1.40	1.35
1	A	135	CFZ	C6-C5	2.10	1.39	1.35
1	A	204	CFZ	C6-C5	2.10	1.39	1.35
1	A	442	CFZ	C6-C5	2.10	1.39	1.35
1	A	609	CFZ	C6-C5	2.10	1.39	1.35
1	A	616	UFT	C4-N3	2.10	1.42	1.38
1	A	153	CFZ	C6-C5	2.10	1.39	1.35
1	A	694	CFZ	C6-C5	2.10	1.39	1.35
1	A	560	CFZ	C6-C5	2.10	1.39	1.35
1	A	374	UFT	C4-N3	2.10	1.42	1.38
1	A	72	CFZ	C6-C5	2.10	1.39	1.35
1	A	438	CFZ	C6-C5	2.10	1.39	1.35
1	A	527	CFZ	C6-C5	2.10	1.39	1.35
1	A	612	UFT	C4-N3	2.09	1.42	1.38
1	A	73	CFZ	C6-C5	2.09	1.39	1.35
1	A	108	CFZ	C6-C5	2.09	1.39	1.35
1	A	167	UFT	C4-N3	2.09	1.42	1.38
1	A	142	UFT	C4-N3	2.09	1.42	1.38
1	A	665	CFZ	C6-C5	2.09	1.39	1.35
1	A	146	CFZ	C6-C5	2.09	1.39	1.35
1	A	23	UFT	C4-N3	2.09	1.42	1.38
1	A	549	UFT	C4-N3	2.09	1.42	1.38
1	A	421	UFT	C4-N3	2.09	1.42	1.38
1	A	378	CFZ	C6-C5	2.08	1.39	1.35
1	A	12	CFZ	C6-C5	2.08	1.39	1.35
1	A	178	CFZ	C6-C5	2.08	1.39	1.35
1	A	340	UFT	C4-N3	2.08	1.42	1.38
1	A	87	CFZ	C6-C5	2.08	1.39	1.35
1	A	269	CFZ	C6-C5	2.08	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	CFZ	C6-C5	2.08	1.39	1.35
1	A	131	CFZ	C6-C5	2.08	1.39	1.35
1	A	219	CFZ	C6-C5	2.08	1.39	1.35
1	A	196	UFT	C4-N3	2.08	1.42	1.38
1	A	95	UFT	C4-N3	2.08	1.42	1.38
1	A	433	CFZ	C6-C5	2.08	1.39	1.35
1	A	589	UFT	C4-N3	2.08	1.42	1.38
1	A	506	CFZ	C6-C5	2.08	1.39	1.35
1	A	182	CFZ	C6-C5	2.08	1.39	1.35
1	A	104	CFZ	C6-C5	2.07	1.39	1.35
1	A	330	CFZ	C6-C5	2.07	1.39	1.35
1	A	499	CFZ	C6-C5	2.07	1.39	1.35
1	A	575	UFT	C4-N3	2.07	1.42	1.38
1	A	156	CFZ	C6-C5	2.07	1.39	1.35
1	A	83	CFZ	C6-C5	2.07	1.39	1.35
1	A	452	CFZ	C6-C5	2.07	1.39	1.35
1	A	641	CFZ	C6-C5	2.07	1.39	1.35
1	A	466	CFZ	C6-C5	2.07	1.39	1.35
1	A	507	UFT	C4-N3	2.07	1.42	1.38
1	A	138	UFT	C4-N3	2.07	1.42	1.38
1	A	437	CFZ	C6-C5	2.07	1.39	1.35
1	A	683	UFT	C4-N3	2.06	1.42	1.38
1	A	116	UFT	C4-N3	2.06	1.42	1.38
1	A	177	UFT	C4-N3	2.06	1.42	1.38
1	A	197	UFT	C4-N3	2.06	1.42	1.38
1	A	476	UFT	C4-N3	2.06	1.42	1.38
1	A	271	CFZ	C6-C5	2.06	1.39	1.35
1	A	541	CFZ	C6-C5	2.06	1.39	1.35
1	A	690	CFZ	C6-C5	2.06	1.39	1.35
1	A	625	CFZ	C6-C5	2.06	1.39	1.35
1	A	355	CFZ	C6-C5	2.06	1.39	1.35
1	A	195	CFZ	C6-C5	2.06	1.39	1.35
1	A	607	UFT	C2'-C1'	-2.06	1.50	1.53
1	A	350	UFT	C4-N3	2.06	1.42	1.38
1	A	617	UFT	C4-N3	2.06	1.42	1.38
1	A	384	CFZ	C6-C5	2.06	1.39	1.35
1	A	115	UFT	C4-N3	2.05	1.42	1.38
1	A	343	CFZ	C6-C5	2.05	1.39	1.35
1	A	19	UFT	C4-N3	2.05	1.42	1.38
1	A	7	CFZ	C6-C5	2.05	1.39	1.35
1	A	369	CFZ	C6-C5	2.05	1.39	1.35
1	A	336	CFZ	C6-C5	2.05	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	UFT	C4-N3	2.05	1.42	1.38
1	A	10	CFZ	C6-C5	2.05	1.39	1.35
1	A	453	CFZ	C6-C5	2.05	1.39	1.35
1	A	42	UFT	C4-N3	2.05	1.42	1.38
1	A	157	CFZ	C6-C5	2.05	1.39	1.35
1	A	563	UFT	C4-N3	2.05	1.42	1.38
1	A	217	CFZ	C6-C5	2.05	1.39	1.35
1	A	76	CFZ	C6-C5	2.05	1.39	1.35
1	A	662	UFT	C4-N3	2.05	1.42	1.38
1	A	630	CFZ	C6-C5	2.05	1.39	1.35
1	A	66	UFT	C4-N3	2.05	1.42	1.38
1	A	190	CFZ	C6-C5	2.05	1.39	1.35
1	A	588	UFT	C4-N3	2.05	1.42	1.38
1	A	344	CFZ	C6-C5	2.04	1.39	1.35
1	A	521	UFT	C4-N3	2.04	1.42	1.38
1	A	493	CFZ	C6-C5	2.04	1.39	1.35
1	A	489	CFZ	C6-C5	2.04	1.39	1.35
1	A	432	CFZ	C6-C5	2.04	1.39	1.35
1	A	310	CFZ	C6-C5	2.04	1.39	1.35
1	A	337	CFZ	C6-C5	2.04	1.39	1.35
1	A	670	UFT	C4-N3	2.04	1.42	1.38
1	A	620	CFZ	C6-C5	2.04	1.39	1.35
1	A	94	UFT	C4-N3	2.04	1.42	1.38
1	A	170	UFT	C4-N3	2.04	1.42	1.38
1	A	75	CFZ	C6-C5	2.04	1.39	1.35
1	A	129	CFZ	C6-C5	2.04	1.39	1.35
1	A	130	CFZ	C6-C5	2.04	1.39	1.35
1	A	422	CFZ	C6-C5	2.04	1.39	1.35
1	A	143	UFT	C4-N3	2.04	1.42	1.38
1	A	345	UFT	C4-N3	2.04	1.42	1.38
1	A	44	UFT	C4-N3	2.04	1.42	1.38
1	A	388	UFT	C4-N3	2.04	1.42	1.38
1	A	658	CFZ	C6-C5	2.04	1.39	1.35
1	A	147	CFZ	C6-C5	2.04	1.39	1.35
1	A	351	UFT	C4-N3	2.04	1.42	1.38
1	A	11	CFZ	C6-C5	2.04	1.39	1.35
1	A	342	CFZ	C6-C5	2.04	1.39	1.35
1	A	547	CFZ	C6-C5	2.04	1.39	1.35
1	A	57	CFZ	C6-C5	2.03	1.39	1.35
1	A	627	UFT	C4-N3	2.03	1.42	1.38
1	A	484	CFZ	C6-C5	2.03	1.39	1.35
1	A	311	UFT	C4-N3	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	CFZ	C6-C5	2.03	1.39	1.35
1	A	512	CFZ	C6-C5	2.03	1.39	1.35
1	A	45	CFZ	C6-C5	2.03	1.39	1.35
1	A	685	CFZ	C6-C5	2.03	1.39	1.35
1	A	314	CFZ	C6-C5	2.03	1.39	1.35
1	A	148	UFT	C4-N3	2.03	1.42	1.38
1	A	238	UFT	C4-N3	2.03	1.42	1.38
1	A	111	CFZ	C6-C5	2.03	1.39	1.35
1	A	585	UFT	C4-N3	2.03	1.42	1.38
1	A	526	CFZ	C6-C5	2.03	1.39	1.35
1	A	127	UFT	C4-N3	2.03	1.42	1.38
1	A	500	CFZ	C6-C5	2.03	1.39	1.35
1	A	504	UFT	C4-N3	2.03	1.42	1.38
1	A	463	CFZ	C6-C5	2.03	1.39	1.35
1	A	463	CFZ	O4'-C4'	2.03	1.49	1.45
1	A	267	UFT	C4-N3	2.03	1.42	1.38
1	A	397	UFT	C4-N3	2.03	1.42	1.38
1	A	41	CFZ	C6-C5	2.03	1.39	1.35
1	A	162	CFZ	C6-C5	2.02	1.39	1.35
1	A	254	UFT	C4-N3	2.02	1.42	1.38
1	A	671	UFT	C4-N3	2.02	1.42	1.38
1	A	698	UFT	C4-N3	2.02	1.42	1.38
1	A	379	CFZ	O4'-C4'	2.02	1.49	1.45
1	A	88	UFT	C4-N3	2.02	1.42	1.38
1	A	137	CFZ	C6-C5	2.02	1.39	1.35
1	A	556	UFT	C4-N3	2.02	1.42	1.38
1	A	46	UFT	C4-N3	2.02	1.42	1.38
1	A	379	CFZ	C6-C5	2.02	1.39	1.35
1	A	276	CFZ	C6-C5	2.02	1.39	1.35
1	A	555	UFT	C4-N3	2.02	1.42	1.38
1	A	287	CFZ	C6-C5	2.02	1.39	1.35
1	A	439	CFZ	C6-C5	2.02	1.39	1.35
1	A	598	CFZ	C6-C5	2.02	1.39	1.35
1	A	28	CFZ	C6-C5	2.02	1.39	1.35
1	A	675	CFZ	C6-C5	2.02	1.39	1.35
1	A	62	UFT	C4-N3	2.02	1.42	1.38
1	A	240	UFT	C4-N3	2.02	1.42	1.38
1	A	274	UFT	C4-N3	2.02	1.42	1.38
1	A	322	UFT	C4-N3	2.01	1.42	1.38
1	A	32	UFT	C4-N3	2.01	1.42	1.38
1	A	485	UFT	C4-N3	2.01	1.42	1.38
1	A	121	CFZ	C6-C5	2.01	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	CFZ	C6-C5	2.01	1.39	1.35
1	A	363	CFZ	C6-C5	2.01	1.39	1.35
1	A	206	CFZ	C6-C5	2.01	1.39	1.35
1	A	175	UFT	C4-N3	2.01	1.42	1.38
1	A	359	CFZ	C6-C5	2.01	1.39	1.35
1	A	597	UFT	C4-N3	2.01	1.42	1.38
1	A	208	CFZ	C6-C5	2.01	1.39	1.35
1	A	288	UFT	C4-N3	2.01	1.42	1.38
1	A	71	UFT	C4-N3	2.00	1.42	1.38

All (1638) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	UFT	C4-N3-C2	-6.80	118.17	126.61
1	A	213	UFT	C4-N3-C2	-6.53	118.51	126.61
1	A	650	UFT	C4-N3-C2	-6.41	118.65	126.61
1	A	56	UFT	C4-N3-C2	-6.32	118.76	126.61
1	A	471	UFT	C4-N3-C2	-6.22	118.89	126.61
1	A	371	UFT	C4-N3-C2	-6.22	118.89	126.61
1	A	559	UFT	C4-N3-C2	-6.19	118.93	126.61
1	A	210	UFT	C4-N3-C2	-6.16	118.97	126.61
1	A	367	UFT	C4-N3-C2	-6.16	118.97	126.61
1	A	303	UFT	C4-N3-C2	-6.15	118.97	126.61
1	A	194	UFT	C4-N3-C2	-6.15	118.98	126.61
1	A	601	UFT	C4-N3-C2	-6.13	119.01	126.61
1	A	595	UFT	C4-N3-C2	-6.10	119.04	126.61
1	A	377	UFT	C4-N3-C2	-6.07	119.08	126.61
1	A	51	UFT	C4-N3-C2	-6.07	119.08	126.61
1	A	638	UFT	C4-N3-C2	-6.05	119.11	126.61
1	A	236	UFT	C4-N3-C2	-6.00	119.16	126.61
1	A	58	UFT	C4-N3-C2	-5.99	119.17	126.61
1	A	283	UFT	C4-N3-C2	-5.92	119.27	126.61
1	A	277	UFT	C4-N3-C2	-5.90	119.29	126.61
1	A	374	UFT	C4-N3-C2	-5.89	119.31	126.61
1	A	687	UFT	C4-N3-C2	-5.86	119.34	126.61
1	A	377	UFT	C2'-C1'-N1	-5.80	105.35	114.27
1	A	550	UFT	C4-N3-C2	-5.79	119.42	126.61
1	A	504	UFT	C4-N3-C2	-5.79	119.43	126.61
1	A	575	UFT	C4-N3-C2	-5.77	119.44	126.61
1	A	464	UFT	C4-N3-C2	-5.76	119.47	126.61
1	A	390	UFT	C4-N3-C2	-5.74	119.49	126.61
1	A	123	UFT	C4-N3-C2	-5.71	119.53	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	UFT	C4-N3-C2	-5.70	119.53	126.61
1	A	66	UFT	C4-N3-C2	-5.70	119.54	126.61
1	A	23	UFT	C4-N3-C2	-5.68	119.56	126.61
1	A	612	UFT	C4-N3-C2	-5.67	119.57	126.61
1	A	311	UFT	C4-N3-C2	-5.66	119.58	126.61
1	A	120	UFT	C4-N3-C2	-5.66	119.59	126.61
1	A	370	UFT	C4-N3-C2	-5.66	119.59	126.61
1	A	44	UFT	C4-N3-C2	-5.65	119.59	126.61
1	A	542	UFT	C4-N3-C2	-5.64	119.61	126.61
1	A	683	UFT	C4-N3-C2	-5.63	119.62	126.61
1	A	356	UFT	C4-N3-C2	-5.63	119.62	126.61
1	A	127	UFT	C4-N3-C2	-5.62	119.63	126.61
1	A	33	UFT	C4-N3-C2	-5.60	119.66	126.61
1	A	693	UFT	C4-N3-C2	-5.60	119.66	126.61
1	A	558	UFT	C4-N3-C2	-5.59	119.67	126.61
1	A	242	UFT	C4-N3-C2	-5.58	119.69	126.61
1	A	230	UFT	C4-N3-C2	-5.57	119.69	126.61
1	A	588	UFT	C4-N3-C2	-5.57	119.70	126.61
1	A	431	UFT	C4-N3-C2	-5.56	119.71	126.61
1	A	361	UFT	C4-N3-C2	-5.54	119.73	126.61
1	A	89	UFT	C4-N3-C2	-5.54	119.74	126.61
1	A	107	UFT	C4-N3-C2	-5.53	119.75	126.61
1	A	597	UFT	C4-N3-C2	-5.53	119.75	126.61
1	A	421	UFT	C4-N3-C2	-5.52	119.75	126.61
1	A	288	UFT	C4-N3-C2	-5.50	119.78	126.61
1	A	476	UFT	C4-N3-C2	-5.50	119.78	126.61
1	A	115	UFT	C4-N3-C2	-5.49	119.80	126.61
1	A	409	UFT	C4-N3-C2	-5.49	119.80	126.61
1	A	589	UFT	C4-N3-C2	-5.48	119.80	126.61
1	A	138	UFT	C4-N3-C2	-5.48	119.81	126.61
1	A	679	UFT	C4-N3-C2	-5.48	119.81	126.61
1	A	142	UFT	C4-N3-C2	-5.48	119.81	126.61
1	A	662	UFT	C4-N3-C2	-5.47	119.82	126.61
1	A	624	UFT	C4-N3-C2	-5.47	119.82	126.61
1	A	95	UFT	C4-N3-C2	-5.46	119.83	126.61
1	A	61	UFT	C4-N3-C2	-5.46	119.84	126.61
1	A	196	UFT	C4-N3-C2	-5.45	119.84	126.61
1	A	644	UFT	C4-N3-C2	-5.45	119.85	126.61
1	A	193	UFT	C4-N3-C2	-5.43	119.87	126.61
1	A	562	UFT	C4-N3-C2	-5.43	119.87	126.61
1	A	340	UFT	C4-N3-C2	-5.42	119.88	126.61
1	A	698	UFT	C4-N3-C2	-5.42	119.88	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	UFT	C4-N3-C2	-5.41	119.89	126.61
1	A	88	UFT	C4-N3-C2	-5.41	119.89	126.61
1	A	590	UFT	C4-N3-C2	-5.41	119.89	126.61
1	A	670	UFT	C4-N3-C2	-5.41	119.90	126.61
1	A	154	UFT	C4-N3-C2	-5.39	119.92	126.61
1	A	93	UFT	C4-N3-C2	-5.39	119.92	126.61
1	A	563	UFT	C4-N3-C2	-5.39	119.92	126.61
1	A	556	UFT	C4-N3-C2	-5.39	119.92	126.61
1	A	616	UFT	C4-N3-C2	-5.39	119.92	126.61
1	A	329	UFT	C4-N3-C2	-5.38	119.93	126.61
1	A	686	UFT	C4-N3-C2	-5.37	119.94	126.61
1	A	345	UFT	C4-N3-C2	-5.36	119.95	126.61
1	A	167	UFT	C4-N3-C2	-5.36	119.96	126.61
1	A	322	UFT	C4-N3-C2	-5.36	119.96	126.61
1	A	6	UFT	C4-N3-C2	-5.36	119.96	126.61
1	A	62	UFT	C4-N3-C2	-5.35	119.97	126.61
1	A	697	UFT	C4-N3-C2	-5.35	119.97	126.61
1	A	397	UFT	C4-N3-C2	-5.34	119.98	126.61
1	A	197	UFT	C4-N3-C2	-5.33	119.99	126.61
1	A	32	UFT	C4-N3-C2	-5.33	119.99	126.61
1	A	143	UFT	C4-N3-C2	-5.33	119.99	126.61
1	A	388	UFT	C4-N3-C2	-5.33	120.00	126.61
1	A	42	UFT	C4-N3-C2	-5.31	120.02	126.61
1	A	94	UFT	C4-N3-C2	-5.31	120.02	126.61
1	A	267	UFT	C4-N3-C2	-5.31	120.02	126.61
1	A	19	UFT	C4-N3-C2	-5.31	120.02	126.61
1	A	667	UFT	C4-N3-C2	-5.30	120.04	126.61
1	A	170	UFT	C4-N3-C2	-5.29	120.04	126.61
1	A	578	CFZ	C3'-C2'-C1'	5.29	109.24	103.10
1	A	617	UFT	C4-N3-C2	-5.28	120.05	126.61
1	A	238	UFT	C4-N3-C2	-5.27	120.07	126.61
1	A	175	UFT	C4-N3-C2	-5.25	120.10	126.61
1	A	485	UFT	C4-N3-C2	-5.24	120.10	126.61
1	A	116	UFT	C4-N3-C2	-5.24	120.10	126.61
1	A	151	UFT	C4-N3-C2	-5.24	120.11	126.61
1	A	585	UFT	C4-N3-C2	-5.23	120.12	126.61
1	A	719	UFT	C4-N3-C2	-5.23	120.12	126.61
1	A	360	UFT	C4-N3-C2	-5.23	120.12	126.61
1	A	521	UFT	C4-N3-C2	-5.23	120.12	126.61
1	A	507	UFT	C4-N3-C2	-5.22	120.13	126.61
1	A	383	UFT	C4-N3-C2	-5.21	120.15	126.61
1	A	350	UFT	C4-N3-C2	-5.20	120.15	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	UFT	C4-N3-C2	-5.20	120.16	126.61
1	A	319	UFT	C4-N3-C2	-5.18	120.18	126.61
1	A	254	UFT	C4-N3-C2	-5.18	120.19	126.61
1	A	339	UFT	C4-N3-C2	-5.17	120.20	126.61
1	A	215	UFT	C4-N3-C2	-5.17	120.20	126.61
1	A	17	UFT	C4-N3-C2	-5.16	120.20	126.61
1	A	643	UFT	C4-N3-C2	-5.16	120.21	126.61
1	A	555	UFT	C4-N3-C2	-5.15	120.22	126.61
1	A	497	UFT	C4-N3-C2	-5.15	120.22	126.61
1	A	169	UFT	C4-N3-C2	-5.14	120.23	126.61
1	A	671	UFT	C4-N3-C2	-5.13	120.24	126.61
1	A	705	UFT	C4-N3-C2	-5.13	120.25	126.61
1	A	716	UFT	C4-N3-C2	-5.12	120.25	126.61
1	A	148	UFT	C4-N3-C2	-5.10	120.28	126.61
1	A	71	UFT	C4-N3-C2	-5.10	120.28	126.61
1	A	655	UFT	C4-N3-C2	-5.09	120.30	126.61
1	A	79	UFT	C4-N3-C2	-5.07	120.32	126.61
1	A	510	UFT	C4-N3-C2	-5.05	120.34	126.61
1	A	177	UFT	C4-N3-C2	-5.05	120.35	126.61
1	A	351	UFT	C4-N3-C2	-5.02	120.38	126.61
1	A	192	UFT	C4-N3-C2	-5.01	120.39	126.61
1	A	573	UFT	C4-N3-C2	-5.00	120.41	126.61
1	A	727	UFT	C4-N3-C2	-4.99	120.42	126.61
1	A	501	UFT	C4-N3-C2	-4.96	120.45	126.61
1	A	444	UFT	C4-N3-C2	-4.96	120.45	126.61
1	A	480	UFT	C4-N3-C2	-4.95	120.47	126.61
1	A	272	UFT	C4-N3-C2	-4.95	120.47	126.61
1	A	46	UFT	C4-N3-C2	-4.94	120.48	126.61
1	A	97	UFT	C4-N3-C2	-4.94	120.48	126.61
1	A	627	UFT	C4-N3-C2	-4.93	120.50	126.61
1	A	377	UFT	C5-C4-N3	4.92	121.69	114.80
1	A	221	UFT	C4-N3-C2	-4.91	120.52	126.61
1	A	48	UFT	C4-N3-C2	-4.90	120.53	126.61
1	A	642	UFT	C4-N3-C2	-4.90	120.53	126.61
1	A	66	UFT	C3'-C2'-C1'	4.90	108.79	103.10
1	A	724	UFT	C4-N3-C2	-4.89	120.55	126.61
1	A	274	UFT	C4-N3-C2	-4.85	120.59	126.61
1	A	177	UFT	C3'-C2'-C1'	4.84	108.72	103.10
1	A	523	UFT	C4-N3-C2	-4.83	120.62	126.61
1	A	621	CFZ	C3'-C2'-C1'	4.83	108.70	103.10
1	A	359	CFZ	C3'-C2'-C1'	4.82	108.69	103.10
1	A	307	UFT	C4-N3-C2	-4.79	120.66	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	CFZ	C3'-C2'-C1'	4.78	108.64	103.10
1	A	377	UFT	C1'-N1-C2	4.75	126.12	117.59
1	A	417	UFT	C4-N3-C2	-4.75	120.72	126.61
1	A	298	UFT	C4-N3-C2	-4.74	120.72	126.61
1	A	391	CFZ	C3'-C2'-C1'	4.74	108.60	103.10
1	A	549	UFT	C4-N3-C2	-4.73	120.74	126.61
1	A	429	UFT	C4-N3-C2	-4.73	120.75	126.61
1	A	497	UFT	C2'-C1'-N1	-4.70	107.05	114.27
1	A	582	UFT	C4-N3-C2	-4.69	120.78	126.61
1	A	607	UFT	N3-C2-N1	4.69	121.00	114.89
1	A	188	UFT	C4-N3-C2	-4.68	120.80	126.61
1	A	468	UFT	C4-N3-C2	-4.67	120.81	126.61
1	A	531	CFZ	C3'-C2'-C1'	4.64	108.49	103.10
1	A	526	CFZ	C3'-C2'-C1'	4.63	108.47	103.10
1	A	419	UFT	C4-N3-C2	-4.60	120.91	126.61
1	A	73	CFZ	C3'-C2'-C1'	4.57	108.40	103.10
1	A	532	UFT	C4-N3-C2	-4.57	120.94	126.61
1	A	515	CFZ	C3'-C2'-C1'	4.56	108.39	103.10
1	A	50	CFZ	C3'-C2'-C1'	4.56	108.39	103.10
1	A	674	CFZ	C3'-C2'-C1'	4.56	108.39	103.10
1	A	346	CFZ	C3'-C2'-C1'	4.56	108.39	103.10
1	A	58	UFT	N3-C2-N1	4.52	120.78	114.89
1	A	11	CFZ	C3'-C2'-C1'	4.50	108.32	103.10
1	A	39	UFT	C4-N3-C2	-4.50	121.03	126.61
1	A	629	CFZ	C2'-C3'-C4'	4.49	108.35	102.43
1	A	713	CFZ	C3'-C2'-C1'	4.48	108.31	103.10
1	A	271	CFZ	C3'-C2'-C1'	4.48	108.30	103.10
1	A	630	CFZ	C3'-C2'-C1'	4.48	108.30	103.10
1	A	527	CFZ	C3'-C2'-C1'	4.47	108.29	103.10
1	A	499	CFZ	C3'-C2'-C1'	4.47	108.29	103.10
1	A	685	CFZ	C3'-C2'-C1'	4.44	108.26	103.10
1	A	256	CFZ	C3'-C2'-C1'	4.43	108.24	103.10
1	A	367	UFT	N3-C2-N1	4.43	120.66	114.89
1	A	169	UFT	C3'-C2'-C1'	4.43	108.24	103.10
1	A	471	UFT	C3'-C2'-C1'	4.43	108.24	103.10
1	A	504	UFT	C3'-C2'-C1'	4.42	108.23	103.10
1	A	213	UFT	N3-C2-N1	4.41	120.63	114.89
1	A	607	UFT	C5-C4-N3	4.41	120.97	114.80
1	A	283	UFT	C2'-C1'-N1	-4.40	107.51	114.27
1	A	504	UFT	N3-C2-N1	4.38	120.59	114.89
1	A	658	CFZ	C3'-C2'-C1'	4.36	108.16	103.10
1	A	171	CFZ	C3'-C2'-C1'	4.35	108.14	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	CFZ	C3'-C2'-C1'	4.35	108.14	103.10
1	A	15	CFZ	C3'-C2'-C1'	4.34	108.14	103.10
1	A	23	UFT	N3-C2-N1	4.34	120.54	114.89
1	A	510	UFT	C3'-C2'-C1'	4.33	108.13	103.10
1	A	650	UFT	N3-C2-N1	4.33	120.53	114.89
1	A	475	UFT	C2'-C3'-C4'	4.33	108.13	102.43
1	A	575	UFT	N3-C2-N1	4.32	120.52	114.89
1	A	582	UFT	C2'-C1'-N1	-4.31	107.64	114.27
1	A	686	UFT	N3-C2-N1	4.30	120.49	114.89
1	A	675	CFZ	C3'-C2'-C1'	4.30	108.09	103.10
1	A	662	UFT	N3-C2-N1	4.29	120.48	114.89
1	A	559	UFT	N3-C2-N1	4.29	120.48	114.89
1	A	717	CFZ	C3'-C2'-C1'	4.29	108.08	103.10
1	A	123	UFT	N3-C2-N1	4.29	120.48	114.89
1	A	367	UFT	C2'-C1'-N1	-4.29	107.68	114.27
1	A	267	UFT	C3'-C2'-C1'	4.28	108.06	103.10
1	A	58	UFT	C2'-C3'-C4'	4.28	108.07	102.43
1	A	210	UFT	N3-C2-N1	4.26	120.44	114.89
1	A	273	CFZ	C3'-C2'-C1'	4.25	108.04	103.10
1	A	650	UFT	C5-C4-N3	4.25	120.75	114.80
1	A	51	UFT	C3'-C2'-C1'	4.24	108.03	103.10
1	A	283	UFT	N3-C2-N1	4.24	120.41	114.89
1	A	359	CFZ	C2'-C3'-C4'	4.24	108.01	102.43
1	A	713	CFZ	C2'-C3'-C4'	4.23	108.01	102.43
1	A	497	UFT	N3-C2-N1	4.23	120.39	114.89
1	A	50	CFZ	C2'-C3'-C4'	4.23	108.00	102.43
1	A	371	UFT	C5-C4-N3	4.22	120.72	114.80
1	A	475	UFT	C4-N3-C2	-4.22	121.37	126.61
1	A	56	UFT	N3-C2-N1	4.21	120.37	114.89
1	A	55	CFZ	C2'-C1'-N1	-4.21	107.80	114.27
1	A	147	CFZ	C3'-C2'-C1'	4.21	107.98	103.10
1	A	374	UFT	N3-C2-N1	4.21	120.37	114.89
1	A	601	UFT	N3-C2-N1	4.20	120.36	114.89
1	A	213	UFT	C5-C4-N3	4.20	120.69	114.80
1	A	288	UFT	N3-C2-N1	4.20	120.36	114.89
1	A	51	UFT	N3-C2-N1	4.20	120.36	114.89
1	A	56	UFT	C5-C4-N3	4.19	120.67	114.80
1	A	311	UFT	N3-C2-N1	4.19	120.34	114.89
1	A	679	UFT	C3'-C2'-C1'	4.19	107.96	103.10
1	A	194	UFT	N3-C2-N1	4.18	120.33	114.89
1	A	371	UFT	N3-C2-N1	4.18	120.33	114.89
1	A	370	UFT	N3-C2-N1	4.18	120.33	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	UFT	N3-C2-N1	4.17	120.32	114.89
1	A	679	UFT	N3-C2-N1	4.17	120.32	114.89
1	A	213	UFT	C3'-C2'-C1'	4.17	107.94	103.10
1	A	501	UFT	N3-C2-N1	4.16	120.31	114.89
1	A	390	UFT	N3-C2-N1	4.16	120.31	114.89
1	A	595	UFT	N3-C2-N1	4.16	120.31	114.89
1	A	665	CFZ	C3'-C2'-C1'	4.16	107.93	103.10
1	A	476	UFT	N3-C2-N1	4.15	120.30	114.89
1	A	154	UFT	N3-C2-N1	4.15	120.29	114.89
1	A	303	UFT	N3-C2-N1	4.15	120.29	114.89
1	A	236	UFT	N3-C2-N1	4.15	120.29	114.89
1	A	618	CFZ	C3'-C2'-C1'	4.14	107.91	103.10
1	A	63	CFZ	C3'-C2'-C1'	4.14	107.91	103.10
1	A	277	UFT	N3-C2-N1	4.14	120.28	114.89
1	A	638	UFT	N3-C2-N1	4.14	120.28	114.89
1	A	603	CFZ	C2'-C3'-C4'	4.14	107.89	102.43
1	A	240	UFT	N3-C2-N1	4.14	120.28	114.89
1	A	588	UFT	N3-C2-N1	4.14	120.28	114.89
1	A	612	UFT	N3-C2-N1	4.14	120.28	114.89
1	A	107	UFT	N3-C2-N1	4.13	120.27	114.89
1	A	178	CFZ	C3'-C2'-C1'	4.13	107.89	103.10
1	A	298	UFT	C2'-C1'-N1	-4.13	107.92	114.27
1	A	378	CFZ	C2'-C3'-C4'	4.13	107.87	102.43
1	A	72	CFZ	C3'-C2'-C1'	4.13	107.89	103.10
1	A	336	CFZ	C3'-C2'-C1'	4.13	107.89	103.10
1	A	573	UFT	C3'-C2'-C1'	4.13	107.89	103.10
1	A	115	UFT	N3-C2-N1	4.12	120.26	114.89
1	A	303	UFT	C5-C4-N3	4.12	120.57	114.80
1	A	65	CFZ	C3'-C2'-C1'	4.11	107.88	103.10
1	A	127	UFT	N3-C2-N1	4.11	120.25	114.89
1	A	356	UFT	N3-C2-N1	4.11	120.25	114.89
1	A	339	UFT	N3-C2-N1	4.11	120.24	114.89
1	A	62	UFT	C3'-C2'-C1'	4.11	107.87	103.10
1	A	322	UFT	N3-C2-N1	4.11	120.24	114.89
1	A	340	UFT	N3-C2-N1	4.11	120.24	114.89
1	A	146	CFZ	C3'-C2'-C1'	4.10	107.86	103.10
1	A	210	UFT	C5-C4-N3	4.10	120.55	114.80
1	A	194	UFT	C5-C4-N3	4.10	120.55	114.80
1	A	471	UFT	C5-C4-N3	4.10	120.55	114.80
1	A	181	UFT	C4-N3-C2	-4.10	121.53	126.61
1	A	431	UFT	N3-C2-N1	4.10	120.23	114.89
1	A	616	UFT	N3-C2-N1	4.10	120.22	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	CFZ	C3'-C2'-C1'	4.10	107.86	103.10
1	A	409	UFT	N3-C2-N1	4.10	120.22	114.89
1	A	693	UFT	N3-C2-N1	4.10	120.22	114.89
1	A	542	UFT	N3-C2-N1	4.09	120.22	114.89
1	A	51	UFT	C5-C4-N3	4.09	120.53	114.80
1	A	444	UFT	N3-C2-N1	4.09	120.22	114.89
1	A	475	UFT	C3'-C2'-C1'	4.09	107.85	103.10
1	A	421	UFT	N3-C2-N1	4.09	120.21	114.89
1	A	624	UFT	N3-C2-N1	4.09	120.21	114.89
1	A	93	UFT	N3-C2-N1	4.09	120.21	114.89
1	A	468	UFT	N3-C2-N1	4.08	120.20	114.89
1	A	33	UFT	N3-C2-N1	4.08	120.20	114.89
1	A	595	UFT	C5-C4-N3	4.08	120.51	114.80
1	A	464	UFT	N3-C2-N1	4.07	120.20	114.89
1	A	556	UFT	N3-C2-N1	4.07	120.19	114.89
1	A	687	UFT	N3-C2-N1	4.07	120.19	114.89
1	A	585	UFT	C3'-C2'-C1'	4.07	107.82	103.10
1	A	658	CFZ	C2'-C3'-C4'	4.07	107.79	102.43
1	A	361	UFT	N3-C2-N1	4.06	120.18	114.89
1	A	335	CFZ	C2'-C3'-C4'	4.06	107.78	102.43
1	A	263	UFT	N3-C2-N1	4.06	120.18	114.89
1	A	44	UFT	N3-C2-N1	4.06	120.18	114.89
1	A	63	CFZ	C2'-C3'-C4'	4.06	107.78	102.43
1	A	109	CFZ	C3'-C2'-C1'	4.06	107.81	103.10
1	A	589	UFT	N3-C2-N1	4.06	120.17	114.89
1	A	19	UFT	N3-C2-N1	4.06	120.17	114.89
1	A	645	CFZ	C3'-C2'-C1'	4.05	107.81	103.10
1	A	267	UFT	N3-C2-N1	4.05	120.17	114.89
1	A	559	UFT	C5-C4-N3	4.05	120.47	114.80
1	A	151	UFT	N3-C2-N1	4.05	120.16	114.89
1	A	562	UFT	N3-C2-N1	4.05	120.16	114.89
1	A	76	CFZ	C2'-C1'-N1	-4.05	108.05	114.27
1	A	510	UFT	N3-C2-N1	4.04	120.15	114.89
1	A	597	UFT	N3-C2-N1	4.04	120.15	114.89
1	A	550	UFT	N3-C2-N1	4.04	120.14	114.89
1	A	175	UFT	N3-C2-N1	4.03	120.14	114.89
1	A	138	UFT	N3-C2-N1	4.03	120.14	114.89
1	A	429	UFT	N3-C2-N1	4.03	120.14	114.89
1	A	71	UFT	N3-C2-N1	4.03	120.14	114.89
1	A	310	CFZ	C3'-C2'-C1'	4.03	107.78	103.10
1	A	256	CFZ	C2'-C3'-C4'	4.03	107.74	102.43
1	A	601	UFT	C5-C4-N3	4.03	120.44	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	UFT	N3-C2-N1	4.03	120.13	114.89
1	A	230	UFT	N3-C2-N1	4.02	120.12	114.89
1	A	272	UFT	N3-C2-N1	4.02	120.12	114.89
1	A	521	UFT	N3-C2-N1	4.01	120.11	114.89
1	A	607	UFT	O4-C4-C5	-4.01	118.25	125.16
1	A	717	CFZ	C2'-C3'-C4'	4.01	107.72	102.43
1	A	417	UFT	N3-C2-N1	4.01	120.11	114.89
1	A	360	UFT	N3-C2-N1	4.01	120.11	114.89
1	A	485	UFT	N3-C2-N1	4.01	120.11	114.89
1	A	547	CFZ	C3'-C2'-C1'	4.00	107.75	103.10
1	A	120	UFT	C3'-C2'-C1'	4.00	107.75	103.10
1	A	705	UFT	N3-C2-N1	4.00	120.10	114.89
1	A	558	UFT	N3-C2-N1	4.00	120.10	114.89
1	A	532	UFT	N3-C2-N1	3.99	120.09	114.89
1	A	656	CFZ	C3'-C2'-C1'	3.99	107.73	103.10
1	A	66	UFT	C5-C4-N3	3.99	120.39	114.80
1	A	170	UFT	N3-C2-N1	3.99	120.08	114.89
1	A	236	UFT	C5-C4-N3	3.99	120.39	114.80
1	A	638	UFT	C5-C4-N3	3.99	120.39	114.80
1	A	230	UFT	C2'-C1'-N1	-3.99	108.14	114.27
1	A	655	UFT	N3-C2-N1	3.98	120.08	114.89
1	A	493	CFZ	C2'-C3'-C4'	3.98	107.68	102.43
1	A	32	UFT	N3-C2-N1	3.98	120.07	114.89
1	A	242	UFT	N3-C2-N1	3.98	120.07	114.89
1	A	515	CFZ	C2'-C3'-C4'	3.98	107.67	102.43
1	A	383	UFT	N3-C2-N1	3.98	120.07	114.89
1	A	219	CFZ	C3'-C2'-C1'	3.97	107.71	103.10
1	A	167	UFT	N3-C2-N1	3.97	120.06	114.89
1	A	727	UFT	N3-C2-N1	3.97	120.06	114.89
1	A	683	UFT	C2'-C3'-C4'	3.97	107.66	102.43
1	A	397	UFT	N3-C2-N1	3.97	120.06	114.89
1	A	582	UFT	N3-C2-N1	3.97	120.06	114.89
1	A	590	UFT	N3-C2-N1	3.97	120.06	114.89
1	A	698	UFT	N3-C2-N1	3.97	120.06	114.89
1	A	468	UFT	C3'-C2'-C1'	3.97	107.70	103.10
1	A	335	CFZ	C3'-C2'-C1'	3.96	107.70	103.10
1	A	670	UFT	N3-C2-N1	3.96	120.05	114.89
1	A	367	UFT	C5-C4-N3	3.96	120.35	114.80
1	A	603	CFZ	C3'-C2'-C1'	3.96	107.69	103.10
1	A	142	UFT	N3-C2-N1	3.96	120.04	114.89
1	A	197	UFT	N3-C2-N1	3.96	120.04	114.89
1	A	17	UFT	N3-C2-N1	3.96	120.04	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	CFZ	C3'-C2'-C1'	3.95	107.69	103.10
1	A	617	UFT	N3-C2-N1	3.95	120.04	114.89
1	A	277	UFT	C5-C4-N3	3.95	120.34	114.80
1	A	120	UFT	N3-C2-N1	3.95	120.03	114.89
1	A	683	UFT	C5-C4-N3	3.95	120.33	114.80
1	A	471	UFT	O4-C4-C5	-3.95	118.35	125.16
1	A	215	UFT	N3-C2-N1	3.95	120.03	114.89
1	A	442	CFZ	C2'-C3'-C4'	3.95	107.63	102.43
1	A	89	UFT	N3-C2-N1	3.95	120.03	114.89
1	A	114	CFZ	C3'-C2'-C1'	3.94	107.68	103.10
1	A	93	UFT	C3'-C2'-C1'	3.94	107.68	103.10
1	A	319	UFT	N3-C2-N1	3.94	120.02	114.89
1	A	42	UFT	N3-C2-N1	3.94	120.02	114.89
1	A	350	UFT	N3-C2-N1	3.94	120.02	114.89
1	A	56	UFT	O4-C4-C5	-3.94	118.37	125.16
1	A	143	UFT	N3-C2-N1	3.94	120.02	114.89
1	A	573	UFT	N3-C2-N1	3.94	120.02	114.89
1	A	687	UFT	C5-C4-N3	3.94	120.31	114.80
1	A	217	CFZ	C3'-C2'-C1'	3.94	107.67	103.10
1	A	563	UFT	N3-C2-N1	3.93	120.01	114.89
1	A	196	UFT	N3-C2-N1	3.93	120.01	114.89
1	A	94	UFT	N3-C2-N1	3.93	120.01	114.89
1	A	667	UFT	N3-C2-N1	3.93	120.01	114.89
1	A	683	UFT	N3-C2-N1	3.93	120.01	114.89
1	A	117	CFZ	C2'-C3'-C4'	3.93	107.61	102.43
1	A	550	UFT	C5-C4-N3	3.93	120.30	114.80
1	A	451	UFT	N3-C2-N1	3.92	120.00	114.89
1	A	345	UFT	N3-C2-N1	3.92	120.00	114.89
1	A	697	UFT	N3-C2-N1	3.92	120.00	114.89
1	A	480	UFT	C2'-C3'-C4'	3.92	107.60	102.43
1	A	374	UFT	C5-C4-N3	3.92	120.29	114.80
1	A	6	UFT	N3-C2-N1	3.92	120.00	114.89
1	A	62	UFT	N3-C2-N1	3.92	120.00	114.89
1	A	107	UFT	C2'-C1'-N1	-3.92	108.25	114.27
1	A	644	UFT	N3-C2-N1	3.92	119.99	114.89
1	A	66	UFT	N3-C2-N1	3.91	119.98	114.89
1	A	409	UFT	C3'-C2'-C1'	3.91	107.64	103.10
1	A	298	UFT	N3-C2-N1	3.91	119.98	114.89
1	A	460	CFZ	C2'-C3'-C4'	3.91	107.59	102.43
1	A	371	UFT	O4-C4-C5	-3.91	118.42	125.16
1	A	88	UFT	N3-C2-N1	3.91	119.98	114.89
1	A	609	CFZ	C3'-C2'-C1'	3.90	107.63	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	UFT	N3-C2-N1	3.90	119.97	114.89
1	A	221	UFT	N3-C2-N1	3.90	119.97	114.89
1	A	120	UFT	C5-C4-N3	3.90	120.26	114.80
1	A	598	CFZ	C3'-C2'-C1'	3.90	107.62	103.10
1	A	716	UFT	C3'-C2'-C1'	3.90	107.62	103.10
1	A	388	UFT	N3-C2-N1	3.90	119.96	114.89
1	A	283	UFT	C5-C4-N3	3.90	120.26	114.80
1	A	148	UFT	N3-C2-N1	3.89	119.96	114.89
1	A	666	CFZ	C3'-C2'-C1'	3.89	107.62	103.10
1	A	95	UFT	N3-C2-N1	3.89	119.95	114.89
1	A	97	UFT	N3-C2-N1	3.88	119.94	114.89
1	A	329	UFT	N3-C2-N1	3.88	119.94	114.89
1	A	507	UFT	N3-C2-N1	3.88	119.94	114.89
1	A	275	CFZ	C3'-C2'-C1'	3.88	107.61	103.10
1	A	116	UFT	N3-C2-N1	3.88	119.94	114.89
1	A	219	CFZ	C2'-C3'-C4'	3.88	107.54	102.43
1	A	94	UFT	C3'-C2'-C1'	3.87	107.59	103.10
1	A	44	UFT	C5-C4-N3	3.87	120.22	114.80
1	A	557	CFZ	C3'-C2'-C1'	3.86	107.59	103.10
1	A	328	CFZ	C2'-C1'-N1	-3.86	108.34	114.27
1	A	645	CFZ	C2'-C3'-C4'	3.86	107.51	102.43
1	A	663	CFZ	C2'-C1'-N1	-3.86	108.34	114.27
1	A	690	CFZ	C3'-C2'-C1'	3.86	107.58	103.10
1	A	499	CFZ	C2'-C3'-C4'	3.85	107.51	102.43
1	A	263	UFT	C5-C4-N3	3.85	120.19	114.80
1	A	407	CFZ	C3'-C2'-C1'	3.84	107.56	103.10
1	A	521	UFT	C3'-C2'-C1'	3.84	107.56	103.10
1	A	75	CFZ	C3'-C2'-C1'	3.84	107.56	103.10
1	A	254	UFT	N3-C2-N1	3.84	119.89	114.89
1	A	550	UFT	O4-C4-C5	-3.84	118.54	125.16
1	A	719	UFT	N3-C2-N1	3.84	119.89	114.89
1	A	419	UFT	C3'-C2'-C1'	3.84	107.56	103.10
1	A	607	UFT	C2'-C1'-N1	-3.84	108.37	114.27
1	A	390	UFT	C5-C4-N3	3.84	120.18	114.80
1	A	193	UFT	N3-C2-N1	3.84	119.89	114.89
1	A	351	UFT	N3-C2-N1	3.84	119.88	114.89
1	A	44	UFT	C3'-C2'-C1'	3.83	107.54	103.10
1	A	360	UFT	C3'-C2'-C1'	3.83	107.54	103.10
1	A	601	UFT	O4-C4-C5	-3.82	118.57	125.16
1	A	79	UFT	N3-C2-N1	3.82	119.87	114.89
1	A	378	CFZ	C3'-C2'-C1'	3.82	107.54	103.10
1	A	58	UFT	C5-C4-N3	3.82	120.15	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	UFT	N3-C2-N1	3.82	119.86	114.89
1	A	671	UFT	N3-C2-N1	3.81	119.86	114.89
1	A	155	CFZ	C3'-C2'-C1'	3.81	107.52	103.10
1	A	89	UFT	C5-C4-N3	3.81	120.14	114.80
1	A	48	UFT	N3-C2-N1	3.81	119.85	114.89
1	A	242	UFT	C5-C4-N3	3.81	120.14	114.80
1	A	370	UFT	C5-C4-N3	3.81	120.13	114.80
1	A	135	CFZ	C2'-C1'-N1	-3.81	108.42	114.27
1	A	575	UFT	C5-C4-N3	3.81	120.13	114.80
1	A	585	UFT	N3-C2-N1	3.81	119.84	114.89
1	A	276	CFZ	C3'-C2'-C1'	3.81	107.52	103.10
1	A	127	UFT	C5-C4-N3	3.80	120.13	114.80
1	A	720	CFZ	C3'-C2'-C1'	3.80	107.52	103.10
1	A	602	CFZ	C3'-C2'-C1'	3.80	107.51	103.10
1	A	594	CFZ	C2'-C3'-C4'	3.80	107.44	102.43
1	A	117	CFZ	C3'-C2'-C1'	3.80	107.51	103.10
1	A	643	UFT	N3-C2-N1	3.80	119.83	114.89
1	A	594	CFZ	C3'-C2'-C1'	3.79	107.50	103.10
1	A	169	UFT	C2'-C3'-C4'	3.79	107.43	102.43
1	A	612	UFT	C5-C4-N3	3.79	120.11	114.80
1	A	165	CFZ	C3'-C2'-C1'	3.79	107.50	103.10
1	A	129	CFZ	C3'-C2'-C1'	3.79	107.50	103.10
1	A	73	CFZ	C2'-C3'-C4'	3.79	107.42	102.43
1	A	181	UFT	C3'-C2'-C1'	3.78	107.49	103.10
1	A	303	UFT	O4-C4-C5	-3.78	118.64	125.16
1	A	339	UFT	C3'-C2'-C1'	3.78	107.49	103.10
1	A	230	UFT	C5-C4-N3	3.78	120.10	114.80
1	A	650	UFT	O4-C4-C5	-3.78	118.64	125.16
1	A	208	CFZ	C3'-C2'-C1'	3.78	107.49	103.10
1	A	627	UFT	N3-C2-N1	3.78	119.81	114.89
1	A	558	UFT	C5-C4-N3	3.77	120.08	114.80
1	A	46	UFT	N3-C2-N1	3.77	119.80	114.89
1	A	642	UFT	N3-C2-N1	3.77	119.80	114.89
1	A	194	UFT	C3'-C2'-C1'	3.77	107.48	103.10
1	A	555	UFT	N3-C2-N1	3.77	119.80	114.89
1	A	666	CFZ	C2'-C3'-C4'	3.77	107.40	102.43
1	A	89	UFT	C2'-C3'-C4'	3.77	107.40	102.43
1	A	188	UFT	N3-C2-N1	3.77	119.80	114.89
1	A	193	UFT	C5-C4-N3	3.77	120.08	114.80
1	A	33	UFT	C5-C4-N3	3.77	120.08	114.80
1	A	242	UFT	C3'-C2'-C1'	3.77	107.47	103.10
1	A	169	UFT	N3-C2-N1	3.77	119.79	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	UFT	C5-C4-N3	3.77	120.08	114.80
1	A	192	UFT	N3-C2-N1	3.76	119.79	114.89
1	A	591	CFZ	C3'-C2'-C1'	3.76	107.47	103.10
1	A	480	UFT	N3-C2-N1	3.76	119.79	114.89
1	A	542	UFT	C5-C4-N3	3.76	120.07	114.80
1	A	693	UFT	C5-C4-N3	3.76	120.07	114.80
1	A	644	UFT	C5-C4-N3	3.76	120.06	114.80
1	A	274	UFT	C3'-C2'-C1'	3.76	107.46	103.10
1	A	643	UFT	C5-C4-N3	3.75	120.06	114.80
1	A	504	UFT	C5-C4-N3	3.75	120.06	114.80
1	A	683	UFT	C3'-C2'-C1'	3.75	107.46	103.10
1	A	88	UFT	C5-C4-N3	3.75	120.05	114.80
1	A	51	UFT	C2'-C3'-C4'	3.75	107.37	102.43
1	A	716	UFT	N3-C2-N1	3.74	119.77	114.89
1	A	138	UFT	C5-C4-N3	3.74	120.04	114.80
1	A	210	UFT	O4-C4-C5	-3.74	118.71	125.16
1	A	188	UFT	C3'-C2'-C1'	3.74	107.44	103.10
1	A	274	UFT	N3-C2-N1	3.74	119.76	114.89
1	A	629	CFZ	C3'-C2'-C1'	3.74	107.44	103.10
1	A	213	UFT	O4-C4-C5	-3.74	118.71	125.16
1	A	679	UFT	C2'-C3'-C4'	3.74	107.35	102.43
1	A	574	CFZ	C2'-C3'-C4'	3.74	107.35	102.43
1	A	590	UFT	C5-C4-N3	3.73	120.03	114.80
1	A	177	UFT	N3-C2-N1	3.73	119.75	114.89
1	A	432	CFZ	C3'-C2'-C1'	3.73	107.43	103.10
1	A	234	CFZ	C3'-C2'-C1'	3.73	107.43	103.10
1	A	522	CFZ	C3'-C2'-C1'	3.73	107.43	103.10
1	A	182	CFZ	C2'-C3'-C4'	3.73	107.34	102.43
1	A	585	UFT	C5-C4-N3	3.73	120.02	114.80
1	A	288	UFT	C3'-C2'-C1'	3.73	107.42	103.10
1	A	61	UFT	C5-C4-N3	3.72	120.02	114.80
1	A	431	UFT	C5-C4-N3	3.72	120.01	114.80
1	A	196	UFT	C3'-C2'-C1'	3.72	107.42	103.10
1	A	464	UFT	C5-C4-N3	3.72	120.01	114.80
1	A	206	CFZ	C3'-C2'-C1'	3.72	107.42	103.10
1	A	94	UFT	C5-C4-N3	3.72	120.01	114.80
1	A	263	UFT	C3'-C2'-C1'	3.72	107.41	103.10
1	A	685	CFZ	C2'-C3'-C4'	3.71	107.33	102.43
1	A	502	CFZ	C4'-O4'-C1'	-3.71	101.27	109.47
1	A	388	UFT	C5-C4-N3	3.71	120.00	114.80
1	A	196	UFT	C5-C4-N3	3.71	120.00	114.80
1	A	670	UFT	C5-C4-N3	3.71	120.00	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	UFT	O4-C4-C5	-3.71	118.77	125.16
1	A	697	UFT	C5-C4-N3	3.70	119.99	114.80
1	A	555	UFT	C5-C4-N3	3.70	119.99	114.80
1	A	421	UFT	C5-C4-N3	3.70	119.98	114.80
1	A	108	CFZ	C2'-C1'-N1	-3.70	108.58	114.27
1	A	23	UFT	C5-C4-N3	3.70	119.98	114.80
1	A	630	CFZ	C2'-C3'-C4'	3.70	107.30	102.43
1	A	656	CFZ	C2'-C3'-C4'	3.70	107.30	102.43
1	A	11	CFZ	C2'-C3'-C4'	3.70	107.30	102.43
1	A	589	UFT	C5-C4-N3	3.69	119.97	114.80
1	A	153	CFZ	C3'-C2'-C1'	3.69	107.39	103.10
1	A	15	CFZ	C2'-C3'-C4'	3.69	107.30	102.43
1	A	562	UFT	C5-C4-N3	3.69	119.97	114.80
1	A	597	UFT	C5-C4-N3	3.69	119.97	114.80
1	A	506	CFZ	C3'-C2'-C1'	3.69	107.38	103.10
1	A	107	UFT	C5-C4-N3	3.69	119.97	114.80
1	A	698	UFT	C5-C4-N3	3.69	119.97	114.80
1	A	345	UFT	C5-C4-N3	3.68	119.96	114.80
1	A	588	UFT	C5-C4-N3	3.68	119.96	114.80
1	A	476	UFT	C5-C4-N3	3.68	119.96	114.80
1	A	671	UFT	C2'-C3'-C4'	3.68	107.28	102.43
1	A	181	UFT	N3-C2-N1	3.68	119.68	114.89
1	A	95	UFT	C5-C4-N3	3.68	119.95	114.80
1	A	169	UFT	C5-C4-N3	3.68	119.95	114.80
1	A	62	UFT	C5-C4-N3	3.68	119.95	114.80
1	A	28	CFZ	C2'-C3'-C4'	3.68	107.28	102.43
1	A	377	UFT	N3-C2-N1	3.68	119.68	114.89
1	A	93	UFT	C5-C4-N3	3.68	119.95	114.80
1	A	679	UFT	C5-C4-N3	3.68	119.95	114.80
1	A	142	UFT	C5-C4-N3	3.67	119.95	114.80
1	A	409	UFT	C5-C4-N3	3.67	119.95	114.80
1	A	716	UFT	C5-C4-N3	3.67	119.95	114.80
1	A	6	UFT	C5-C4-N3	3.67	119.95	114.80
1	A	344	CFZ	C3'-C2'-C1'	3.67	107.36	103.10
1	A	728	CFZ	C3'-C2'-C1'	3.67	107.36	103.10
1	A	590	UFT	C2'-C3'-C4'	3.67	107.27	102.43
1	A	719	UFT	C3'-C2'-C1'	3.67	107.36	103.10
1	A	97	UFT	C2'-C1'-N1	-3.67	108.64	114.27
1	A	591	CFZ	C2'-C3'-C4'	3.67	107.26	102.43
1	A	559	UFT	O4-C4-C5	-3.67	118.84	125.16
1	A	123	UFT	C5-C4-N3	3.66	119.93	114.80
1	A	32	UFT	C5-C4-N3	3.66	119.93	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	UFT	C5-C4-N3	3.66	119.92	114.80
1	A	719	UFT	C5-C4-N3	3.66	119.92	114.80
1	A	638	UFT	O4-C4-C5	-3.65	118.86	125.16
1	A	649	CFZ	C3'-C2'-C1'	3.65	107.34	103.10
1	A	356	UFT	C5-C4-N3	3.65	119.91	114.80
1	A	345	UFT	C2'-C3'-C4'	3.65	107.24	102.43
1	A	523	UFT	N3-C2-N1	3.65	119.64	114.89
1	A	397	UFT	C5-C4-N3	3.65	119.91	114.80
1	A	307	UFT	N3-C2-N1	3.64	119.64	114.89
1	A	115	UFT	C5-C4-N3	3.64	119.90	114.80
1	A	192	UFT	C5-C4-N3	3.64	119.90	114.80
1	A	667	UFT	C5-C4-N3	3.64	119.90	114.80
1	A	116	UFT	C5-C4-N3	3.64	119.90	114.80
1	A	177	UFT	C5-C4-N3	3.64	119.90	114.80
1	A	624	UFT	C5-C4-N3	3.64	119.89	114.80
1	A	197	UFT	C5-C4-N3	3.64	119.89	114.80
1	A	148	UFT	C5-C4-N3	3.63	119.89	114.80
1	A	171	CFZ	C2'-C3'-C4'	3.63	107.22	102.43
1	A	238	UFT	C5-C4-N3	3.63	119.89	114.80
1	A	442	CFZ	C3'-C2'-C1'	3.63	107.31	103.10
1	A	322	UFT	C2'-C1'-N1	-3.63	108.69	114.27
1	A	17	UFT	C5-C4-N3	3.63	119.88	114.80
1	A	329	UFT	C5-C4-N3	3.63	119.88	114.80
1	A	143	UFT	C5-C4-N3	3.62	119.88	114.80
1	A	19	UFT	C2'-C1'-N1	-3.62	108.70	114.27
1	A	370	UFT	C3'-C2'-C1'	3.62	107.30	103.10
1	A	437	CFZ	C3'-C2'-C1'	3.62	107.30	103.10
1	A	167	UFT	C5-C4-N3	3.61	119.86	114.80
1	A	170	UFT	C5-C4-N3	3.61	119.86	114.80
1	A	288	UFT	C5-C4-N3	3.61	119.86	114.80
1	A	42	UFT	C5-C4-N3	3.61	119.86	114.80
1	A	527	CFZ	C2'-C3'-C4'	3.61	107.19	102.43
1	A	507	UFT	C5-C4-N3	3.61	119.85	114.80
1	A	175	UFT	C5-C4-N3	3.61	119.85	114.80
1	A	350	UFT	C5-C4-N3	3.61	119.85	114.80
1	A	319	UFT	C3'-C2'-C1'	3.61	107.28	103.10
1	A	616	UFT	C5-C4-N3	3.60	119.85	114.80
1	A	101	CFZ	C3'-C2'-C1'	3.60	107.28	103.10
1	A	383	UFT	C5-C4-N3	3.60	119.84	114.80
1	A	595	UFT	O4-C4-C5	-3.60	118.95	125.16
1	A	556	UFT	C5-C4-N3	3.60	119.84	114.80
1	A	724	UFT	C2'-C3'-C4'	3.60	107.17	102.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	UFT	O4-C4-C5	-3.60	118.96	125.16
1	A	322	UFT	C5-C4-N3	3.60	119.84	114.80
1	A	254	UFT	C5-C4-N3	3.59	119.83	114.80
1	A	147	CFZ	C2'-C3'-C4'	3.59	107.17	102.43
1	A	267	UFT	C5-C4-N3	3.59	119.83	114.80
1	A	19	UFT	C5-C4-N3	3.59	119.83	114.80
1	A	671	UFT	C3'-C2'-C1'	3.59	107.27	103.10
1	A	153	CFZ	C2'-C3'-C4'	3.59	107.16	102.43
1	A	671	UFT	C5-C4-N3	3.59	119.82	114.80
1	A	637	CFZ	C3'-C2'-C1'	3.59	107.26	103.10
1	A	617	UFT	C2'-C3'-C4'	3.59	107.16	102.43
1	A	531	CFZ	C2'-C3'-C4'	3.59	107.16	102.43
1	A	386	CFZ	C2'-C1'-N1	-3.58	108.76	114.27
1	A	46	UFT	C5-C4-N3	3.58	119.82	114.80
1	A	240	UFT	C5-C4-N3	3.58	119.81	114.80
1	A	627	UFT	C5-C4-N3	3.58	119.81	114.80
1	A	90	CFZ	C3'-C2'-C1'	3.58	107.25	103.10
1	A	88	UFT	C3'-C2'-C1'	3.58	107.25	103.10
1	A	215	UFT	C5-C4-N3	3.57	119.81	114.80
1	A	617	UFT	C5-C4-N3	3.57	119.80	114.80
1	A	613	CFZ	C3'-C2'-C1'	3.57	107.25	103.10
1	A	417	UFT	C2'-C1'-N1	-3.57	108.78	114.27
1	A	662	UFT	C5-C4-N3	3.57	119.80	114.80
1	A	111	CFZ	C3'-C2'-C1'	3.57	107.24	103.10
1	A	556	UFT	C2'-C1'-N1	-3.57	108.79	114.27
1	A	155	CFZ	C2'-C3'-C4'	3.57	107.13	102.43
1	A	45	CFZ	C3'-C2'-C1'	3.56	107.24	103.10
1	A	302	CFZ	C3'-C2'-C1'	3.56	107.24	103.10
1	A	361	UFT	C5-C4-N3	3.56	119.79	114.80
1	A	650	UFT	C3'-C2'-C1'	3.56	107.23	103.10
1	A	319	UFT	C5-C4-N3	3.56	119.78	114.80
1	A	674	CFZ	C2'-C3'-C4'	3.56	107.12	102.43
1	A	416	CFZ	C3'-C2'-C1'	3.56	107.23	103.10
1	A	154	UFT	C5-C4-N3	3.56	119.78	114.80
1	A	431	UFT	C3'-C2'-C1'	3.55	107.23	103.10
1	A	557	CFZ	C2'-C3'-C4'	3.55	107.11	102.43
1	A	369	CFZ	C3'-C2'-C1'	3.55	107.22	103.10
1	A	601	UFT	C3'-C2'-C1'	3.55	107.22	103.10
1	A	356	UFT	C3'-C2'-C1'	3.54	107.21	103.10
1	A	487	CFZ	C3'-C2'-C1'	3.54	107.21	103.10
1	A	451	UFT	C5-C4-N3	3.54	119.76	114.80
1	A	485	UFT	C5-C4-N3	3.54	119.76	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	CFZ	C3'-C2'-C1'	3.54	107.21	103.10
1	A	549	UFT	N3-C2-N1	3.54	119.50	114.89
1	A	362	CFZ	C3'-C2'-C1'	3.53	107.20	103.10
1	A	151	UFT	C5-C4-N3	3.53	119.75	114.80
1	A	157	CFZ	C3'-C2'-C1'	3.53	107.19	103.10
1	A	618	CFZ	C2'-C3'-C4'	3.52	107.07	102.43
1	A	322	UFT	C3'-C2'-C1'	3.52	107.19	103.10
1	A	549	UFT	C5-C4-N3	3.52	119.73	114.80
1	A	521	UFT	C5-C4-N3	3.52	119.73	114.80
1	A	661	CFZ	C3'-C2'-C1'	3.52	107.19	103.10
1	A	182	CFZ	C3'-C2'-C1'	3.52	107.18	103.10
1	A	501	UFT	C3'-C2'-C1'	3.52	107.18	103.10
1	A	277	UFT	C3'-C2'-C1'	3.52	107.18	103.10
1	A	642	UFT	C5-C4-N3	3.52	119.72	114.80
1	A	675	CFZ	C2'-C3'-C4'	3.51	107.06	102.43
1	A	340	UFT	C5-C4-N3	3.51	119.72	114.80
1	A	397	UFT	C3'-C2'-C1'	3.51	107.17	103.10
1	A	709	CFZ	C3'-C2'-C1'	3.51	107.17	103.10
1	A	687	UFT	O4-C4-C5	-3.51	119.11	125.16
1	A	523	UFT	C5-C4-N3	3.51	119.71	114.80
1	A	123	UFT	C3'-C2'-C1'	3.51	107.17	103.10
1	A	79	UFT	C5-C4-N3	3.50	119.70	114.80
1	A	12	CFZ	C3'-C2'-C1'	3.50	107.16	103.10
1	A	233	CFZ	C3'-C2'-C1'	3.50	107.16	103.10
1	A	90	CFZ	C2'-C3'-C4'	3.50	107.04	102.43
1	A	330	CFZ	C3'-C2'-C1'	3.50	107.16	103.10
1	A	198	CFZ	C2'-C1'-N1	-3.49	108.90	114.27
1	A	390	UFT	C3'-C2'-C1'	3.49	107.15	103.10
1	A	137	CFZ	C3'-C2'-C1'	3.49	107.15	103.10
1	A	329	UFT	C3'-C2'-C1'	3.49	107.15	103.10
1	A	39	UFT	N3-C2-N1	3.49	119.43	114.89
1	A	480	UFT	C5-C4-N3	3.48	119.68	114.80
1	A	350	UFT	C3'-C2'-C1'	3.48	107.14	103.10
1	A	588	UFT	C3'-C2'-C1'	3.48	107.14	103.10
1	A	307	UFT	C5-C4-N3	3.48	119.67	114.80
1	A	114	CFZ	C2'-C3'-C4'	3.48	107.01	102.43
1	A	95	UFT	C3'-C2'-C1'	3.48	107.14	103.10
1	A	573	UFT	C5-C4-N3	3.47	119.66	114.80
1	A	419	UFT	N3-C2-N1	3.47	119.40	114.89
1	A	600	CFZ	C3'-C2'-C1'	3.46	107.12	103.10
1	A	686	UFT	C5-C4-N3	3.46	119.65	114.80
1	A	705	UFT	C5-C4-N3	3.46	119.65	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	CFZ	C3'-C2'-C1'	3.46	107.12	103.10
1	A	360	UFT	C5-C4-N3	3.46	119.64	114.80
1	A	727	UFT	C5-C4-N3	3.46	119.64	114.80
1	A	382	CFZ	C3'-C2'-C1'	3.46	107.11	103.10
1	A	95	UFT	C2'-C3'-C4'	3.46	106.99	102.43
1	A	475	UFT	C5-C4-N3	3.46	119.64	114.80
1	A	283	UFT	O4-C4-C5	-3.45	119.20	125.16
1	A	97	UFT	C5-C4-N3	3.45	119.64	114.80
1	A	190	CFZ	C3'-C2'-C1'	3.45	107.11	103.10
1	A	433	CFZ	C3'-C2'-C1'	3.45	107.11	103.10
1	A	512	CFZ	C3'-C2'-C1'	3.45	107.11	103.10
1	A	62	UFT	C2'-C3'-C4'	3.45	106.98	102.43
1	A	195	CFZ	C3'-C2'-C1'	3.45	107.11	103.10
1	A	71	UFT	C5-C4-N3	3.45	119.63	114.80
1	A	66	UFT	O4-C4-C5	-3.45	119.21	125.16
1	A	351	UFT	C5-C4-N3	3.45	119.63	114.80
1	A	558	UFT	O4-C4-C5	-3.45	119.22	125.16
1	A	388	UFT	C3'-C2'-C1'	3.45	107.10	103.10
1	A	339	UFT	C5-C4-N3	3.45	119.63	114.80
1	A	655	UFT	C5-C4-N3	3.44	119.62	114.80
1	A	419	UFT	C5-C4-N3	3.44	119.62	114.80
1	A	236	UFT	O4-C4-C5	-3.44	119.23	125.16
1	A	277	UFT	C2'-C3'-C4'	3.44	106.96	102.43
1	A	48	UFT	C5-C4-N3	3.44	119.61	114.80
1	A	635	CFZ	C3'-C2'-C1'	3.44	107.09	103.10
1	A	302	CFZ	C2'-C3'-C4'	3.44	106.96	102.43
1	A	426	CFZ	C3'-C2'-C1'	3.43	107.08	103.10
1	A	510	UFT	C5-C4-N3	3.43	119.60	114.80
1	A	395	CFZ	C2'-C1'-N1	-3.43	109.01	114.27
1	A	277	UFT	O4-C4-C5	-3.42	119.27	125.16
1	A	215	UFT	C3'-C2'-C1'	3.42	107.07	103.10
1	A	79	UFT	C3'-C2'-C1'	3.42	107.07	103.10
1	A	274	UFT	C5-C4-N3	3.42	119.58	114.80
1	A	409	UFT	C2'-C3'-C4'	3.41	106.93	102.43
1	A	475	UFT	C1'-N1-C2	3.41	123.72	117.59
1	A	221	UFT	C5-C4-N3	3.41	119.57	114.80
1	A	212	CFZ	C3'-C2'-C1'	3.41	107.06	103.10
1	A	184	CFZ	C2'-C3'-C4'	3.41	106.92	102.43
1	A	311	UFT	C2'-C3'-C4'	3.41	106.92	102.43
1	A	188	UFT	C5-C4-N3	3.41	119.57	114.80
1	A	597	UFT	C3'-C2'-C1'	3.40	107.05	103.10
1	A	340	UFT	C2'-C1'-N1	-3.40	109.05	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	UFT	C2'-C3'-C4'	3.39	106.90	102.43
1	A	547	CFZ	C2'-C3'-C4'	3.39	106.90	102.43
1	A	391	CFZ	C2'-C3'-C4'	3.39	106.90	102.43
1	A	683	UFT	O4-C4-C5	-3.39	119.32	125.16
1	A	585	UFT	C2'-C3'-C4'	3.39	106.90	102.43
1	A	698	UFT	C2'-C3'-C4'	3.39	106.89	102.43
1	A	476	UFT	C3'-C2'-C1'	3.39	107.03	103.10
1	A	502	CFZ	C3'-C2'-C1'	3.39	107.03	103.10
1	A	39	UFT	C5-C4-N3	3.39	119.54	114.80
1	A	532	UFT	C3'-C2'-C1'	3.38	107.03	103.10
1	A	374	UFT	C2'-C3'-C4'	3.38	106.89	102.43
1	A	367	UFT	O4-C4-C5	-3.38	119.33	125.16
1	A	269	CFZ	C3'-C2'-C1'	3.38	107.02	103.10
1	A	464	UFT	C3'-C2'-C1'	3.38	107.02	103.10
1	A	120	UFT	O4-C4-C5	-3.37	119.34	125.16
1	A	128	CFZ	C3'-C2'-C1'	3.37	107.01	103.10
1	A	329	UFT	C2'-C1'-N1	-3.36	109.10	114.27
1	A	274	UFT	C2'-C3'-C4'	3.36	106.86	102.43
1	A	7	CFZ	C2'-C1'-N1	-3.36	109.10	114.27
1	A	467	CFZ	C3'-C2'-C1'	3.36	107.00	103.10
1	A	138	UFT	C3'-C2'-C1'	3.36	107.00	103.10
1	A	497	UFT	C5-C4-N3	3.35	119.49	114.80
1	A	655	UFT	C2'-C3'-C4'	3.35	106.84	102.43
1	A	485	UFT	C3'-C2'-C1'	3.35	106.99	103.10
1	A	542	UFT	C3'-C2'-C1'	3.35	106.99	103.10
1	A	120	UFT	C2'-C3'-C4'	3.35	106.84	102.43
1	A	170	UFT	C2'-C1'-N1	-3.33	109.15	114.27
1	A	276	CFZ	C2'-C3'-C4'	3.33	106.82	102.43
1	A	617	UFT	C3'-C2'-C1'	3.33	106.96	103.10
1	A	542	UFT	O4-C4-C5	-3.33	119.42	125.16
1	A	629	CFZ	O2-C2-N3	-3.33	117.08	122.33
1	A	343	CFZ	C3'-C2'-C1'	3.33	106.96	103.10
1	A	26	CFZ	C3'-C2'-C1'	3.32	106.95	103.10
1	A	81	CFZ	C2'-C1'-N1	-3.32	109.17	114.27
1	A	154	UFT	C3'-C2'-C1'	3.32	106.95	103.10
1	A	193	UFT	O4-C4-C5	-3.31	119.44	125.16
1	A	392	CFZ	C2'-C1'-N1	-3.31	109.18	114.27
1	A	480	UFT	C3'-C2'-C1'	3.31	106.94	103.10
1	A	631	CFZ	C3'-C2'-C1'	3.31	106.94	103.10
1	A	562	UFT	C3'-C2'-C1'	3.31	106.94	103.10
1	A	573	UFT	C1'-N1-C2	3.30	123.53	117.59
1	A	421	UFT	C2'-C1'-N1	-3.30	109.19	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	UFT	C2'-C1'-N1	-3.30	109.20	114.27
1	A	665	CFZ	C2'-C3'-C4'	3.30	106.78	102.43
1	A	361	UFT	F2'-C2'-C3'	3.30	115.65	109.14
1	A	93	UFT	O4-C4-C5	-3.30	119.48	125.16
1	A	351	UFT	C3'-C2'-C1'	3.29	106.92	103.10
1	A	366	CFZ	C3'-C2'-C1'	3.29	106.92	103.10
1	A	240	UFT	C3'-C2'-C1'	3.29	106.92	103.10
1	A	641	CFZ	C2'-C1'-N1	-3.29	109.22	114.27
1	A	601	UFT	C2'-C1'-N1	-3.29	109.22	114.27
1	A	598	CFZ	C2'-C3'-C4'	3.29	106.76	102.43
1	A	559	UFT	C3'-C2'-C1'	3.28	106.91	103.10
1	A	272	UFT	C5-C4-N3	3.28	119.39	114.80
1	A	510	UFT	C2'-C3'-C4'	3.28	106.75	102.43
1	A	638	UFT	C3'-C2'-C1'	3.28	106.90	103.10
1	A	184	CFZ	C3'-C2'-C1'	3.27	106.90	103.10
1	A	624	UFT	C3'-C2'-C1'	3.27	106.90	103.10
1	A	194	UFT	C2'-C3'-C4'	3.27	106.74	102.43
1	A	56	UFT	C3'-C2'-C1'	3.27	106.90	103.10
1	A	263	UFT	O4-C4-C5	-3.27	119.52	125.16
1	A	444	UFT	C5-C4-N3	3.27	119.38	114.80
1	A	667	UFT	C2'-C3'-C4'	3.26	106.73	102.43
1	A	582	UFT	C5-C4-N3	3.26	119.37	114.80
1	A	44	UFT	O4-C4-C5	-3.26	119.54	125.16
1	A	58	UFT	O2-C2-N1	-3.26	118.56	122.80
1	A	563	UFT	C3'-C2'-C1'	3.26	106.88	103.10
1	A	395	CFZ	C3'-C2'-C1'	3.26	106.88	103.10
1	A	720	CFZ	C2'-C3'-C4'	3.25	106.72	102.43
1	A	501	UFT	C5-C4-N3	3.25	119.36	114.80
1	A	384	CFZ	C2'-C1'-N1	-3.25	109.28	114.27
1	A	667	UFT	C3'-C2'-C1'	3.25	106.87	103.10
1	A	612	UFT	O4-C4-C5	-3.24	119.57	125.16
1	A	298	UFT	C5-C4-N3	3.24	119.34	114.80
1	A	101	CFZ	C2'-C3'-C4'	3.24	106.70	102.43
1	A	275	CFZ	C2'-C3'-C4'	3.24	106.70	102.43
1	A	374	UFT	O4-C4-C5	-3.24	119.58	125.16
1	A	314	CFZ	C3'-C2'-C1'	3.24	106.86	103.10
1	A	693	UFT	O4-C4-C5	-3.23	119.59	125.16
1	A	204	CFZ	C3'-C2'-C1'	3.23	106.85	103.10
1	A	390	UFT	O4-C4-C5	-3.23	119.59	125.16
1	A	620	CFZ	C3'-C2'-C1'	3.23	106.85	103.10
1	A	694	CFZ	C3'-C2'-C1'	3.23	106.85	103.10
1	A	272	UFT	C2'-C1'-N1	-3.23	109.31	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	UFT	C2'-C3'-C4'	3.22	106.68	102.43
1	A	388	UFT	C2'-C3'-C4'	3.22	106.68	102.43
1	A	709	CFZ	C1'-N1-C2	3.21	125.54	118.44
1	A	724	UFT	C5-C4-N3	3.21	119.29	114.80
1	A	165	CFZ	C2'-C3'-C4'	3.21	106.66	102.43
1	A	453	CFZ	C2'-C1'-N1	-3.21	109.34	114.27
1	A	690	CFZ	C2'-C3'-C4'	3.20	106.65	102.43
1	A	456	CFZ	C3'-C2'-C1'	3.20	106.82	103.10
1	A	716	UFT	O4-C4-C5	-3.20	119.65	125.16
1	A	94	UFT	O4-C4-C5	-3.19	119.66	125.16
1	A	142	UFT	C2'-C3'-C4'	3.19	106.64	102.43
1	A	699	CFZ	C3'-C2'-C1'	3.19	106.80	103.10
1	A	303	UFT	C3'-C2'-C1'	3.19	106.80	103.10
1	A	108	CFZ	C3'-C2'-C1'	3.18	106.80	103.10
1	A	696	CFZ	C2'-C1'-N1	-3.18	109.38	114.27
1	A	307	UFT	C3'-C2'-C1'	3.18	106.79	103.10
1	A	468	UFT	C5-C4-N3	3.18	119.25	114.80
1	A	94	UFT	C1'-N1-C2	3.17	123.29	117.59
1	A	87	CFZ	C2'-C1'-N1	-3.17	109.39	114.27
1	A	355	CFZ	C3'-C2'-C1'	3.17	106.78	103.10
1	A	377	UFT	C1'-N1-C6	-3.17	114.01	120.78
1	A	386	CFZ	C3'-C2'-C1'	3.17	106.77	103.10
1	A	662	UFT	C3'-C2'-C1'	3.16	106.77	103.10
1	A	23	UFT	O4-C4-C5	-3.16	119.71	125.16
1	A	33	UFT	O4-C4-C5	-3.16	119.71	125.16
1	A	458	CFZ	C3'-C2'-C1'	3.16	106.77	103.10
1	A	504	UFT	O4-C4-C5	-3.16	119.71	125.16
1	A	627	UFT	C2'-C1'-N1	-3.16	109.42	114.27
1	A	109	CFZ	C2'-C3'-C4'	3.16	106.59	102.43
1	A	601	UFT	C2'-C3'-C4'	3.16	106.59	102.43
1	A	500	CFZ	C2'-C3'-C4'	3.15	106.58	102.43
1	A	695	CFZ	C3'-C2'-C1'	3.15	106.76	103.10
1	A	95	UFT	O4-C4-C5	-3.15	119.73	125.16
1	A	356	UFT	O4-C4-C5	-3.15	119.73	125.16
1	A	115	UFT	C2'-C1'-N1	-3.15	109.43	114.27
1	A	409	UFT	O4-C4-C5	-3.14	119.74	125.16
1	A	631	CFZ	C2'-C1'-N1	-3.14	109.44	114.27
1	A	94	UFT	C2'-C3'-C4'	3.14	106.57	102.43
1	A	526	CFZ	C2'-C3'-C4'	3.14	106.57	102.43
1	A	212	CFZ	C2'-C3'-C4'	3.14	106.56	102.43
1	A	655	UFT	C3'-C2'-C1'	3.14	106.74	103.10
1	A	667	UFT	O4-C4-C5	-3.14	119.75	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	CFZ	C2'-C1'-N1	-3.14	109.45	114.27
1	A	724	UFT	C3'-C2'-C1'	3.13	106.74	103.10
1	A	242	UFT	O4-C4-C5	-3.13	119.76	125.16
1	A	464	UFT	O4-C4-C5	-3.13	119.76	125.16
1	A	564	CFZ	C3'-C2'-C1'	3.13	106.73	103.10
1	A	417	UFT	C5-C4-N3	3.13	119.18	114.80
1	A	10	CFZ	C2'-C1'-N1	-3.13	109.46	114.27
1	A	130	CFZ	C3'-C2'-C1'	3.13	106.73	103.10
1	A	518	CFZ	C3'-C2'-C1'	3.13	106.73	103.10
1	A	310	CFZ	C2'-C3'-C4'	3.12	106.55	102.43
1	A	577	CFZ	C3'-C2'-C1'	3.12	106.73	103.10
1	A	61	UFT	C2'-C1'-N1	-3.12	109.47	114.27
1	A	93	UFT	C2'-C3'-C4'	3.12	106.55	102.43
1	A	217	CFZ	C2'-C3'-C4'	3.12	106.54	102.43
1	A	523	UFT	C3'-C2'-C1'	3.12	106.72	103.10
1	A	556	UFT	C3'-C2'-C1'	3.12	106.72	103.10
1	A	663	CFZ	C3'-C2'-C1'	3.12	106.72	103.10
1	A	452	CFZ	C3'-C2'-C1'	3.12	106.72	103.10
1	A	127	UFT	C3'-C2'-C1'	3.11	106.71	103.10
1	A	575	UFT	O4-C4-C5	-3.11	119.80	125.16
1	A	58	UFT	O4-C4-C5	-3.11	119.80	125.16
1	A	272	UFT	C3'-C2'-C1'	3.11	106.71	103.10
1	A	236	UFT	C3'-C2'-C1'	3.11	106.70	103.10
1	A	429	UFT	C5-C4-N3	3.10	119.14	114.80
1	A	175	UFT	O4-C4-C5	-3.10	119.81	125.16
1	A	157	CFZ	C2'-C1'-N1	-3.10	109.51	114.27
1	A	230	UFT	O4-C4-C5	-3.10	119.82	125.16
1	A	267	UFT	C2'-C3'-C4'	3.10	106.51	102.43
1	A	466	CFZ	C3'-C2'-C1'	3.09	106.69	103.10
1	A	314	CFZ	C2'-C3'-C4'	3.09	106.51	102.43
1	A	657	CFZ	C2'-C3'-C4'	3.09	106.51	102.43
1	A	177	UFT	O4-C4-C5	-3.09	119.83	125.16
1	A	336	CFZ	C2'-C3'-C4'	3.09	106.51	102.43
1	A	555	UFT	C2'-C1'-N1	-3.09	109.52	114.27
1	A	221	UFT	C3'-C2'-C1'	3.09	106.69	103.10
1	A	510	UFT	C2'-C1'-N1	-3.09	109.52	114.27
1	A	44	UFT	C2'-C3'-C4'	3.09	106.50	102.43
1	A	197	UFT	C3'-C2'-C1'	3.08	106.68	103.10
1	A	361	UFT	O4-C4-C5	-3.08	119.85	125.16
1	A	728	CFZ	C2'-C3'-C4'	3.08	106.49	102.43
1	A	521	UFT	O4-C4-C5	-3.08	119.86	125.16
1	A	521	UFT	C2'-C1'-N1	-3.07	109.55	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	UFT	O4-C4-C5	-3.07	119.87	125.16
1	A	697	UFT	C2'-C1'-N1	-3.07	109.55	114.27
1	A	532	UFT	C5-C4-N3	3.07	119.09	114.80
1	A	546	CFZ	C3'-C2'-C1'	3.06	106.66	103.10
1	A	549	UFT	C3'-C2'-C1'	3.06	106.66	103.10
1	A	595	UFT	C3'-C2'-C1'	3.06	106.66	103.10
1	A	342	CFZ	C3'-C2'-C1'	3.06	106.65	103.10
1	A	371	UFT	C2'-C1'-N1	-3.06	109.57	114.27
1	A	632	CFZ	C3'-C2'-C1'	3.06	106.65	103.10
1	A	515	CFZ	C1'-N1-C2	3.06	125.19	118.44
1	A	127	UFT	C2'-C3'-C4'	3.06	106.46	102.43
1	A	61	UFT	O4-C4-C5	-3.05	119.90	125.16
1	A	590	UFT	C3'-C2'-C1'	3.05	106.64	103.10
1	A	32	UFT	C2'-C1'-N1	-3.05	109.59	114.27
1	A	142	UFT	C3'-C2'-C1'	3.05	106.64	103.10
1	A	116	UFT	O4-C4-C5	-3.05	119.91	125.16
1	A	500	CFZ	C4'-O4'-C1'	-3.04	102.75	109.47
1	A	431	UFT	O4-C4-C5	-3.04	119.92	125.16
1	A	169	UFT	O4-C4-C5	-3.04	119.92	125.16
1	A	643	UFT	O4-C4-C5	-3.04	119.92	125.16
1	A	422	CFZ	C2'-C1'-N1	-3.04	109.60	114.27
1	A	271	CFZ	C2'-C3'-C4'	3.04	106.44	102.43
1	A	137	CFZ	C2'-C3'-C4'	3.04	106.44	102.43
1	A	650	UFT	C2'-C3'-C4'	3.04	106.43	102.43
1	A	555	UFT	O4-C4-C5	-3.04	119.92	125.16
1	A	17	UFT	C2'-C1'-N1	-3.03	109.61	114.27
1	A	699	CFZ	C2'-C3'-C4'	3.03	106.43	102.43
1	A	686	UFT	C3'-C2'-C1'	3.03	106.62	103.10
1	A	42	UFT	O4-C4-C5	-3.03	119.93	125.16
1	A	151	UFT	C3'-C2'-C1'	3.03	106.62	103.10
1	A	679	UFT	O4-C4-C5	-3.03	119.94	125.16
1	A	71	UFT	C1'-N1-C2	3.03	123.03	117.59
1	A	561	CFZ	C2'-C1'-N1	-3.03	109.62	114.27
1	A	167	UFT	C3'-C2'-C1'	3.02	106.61	103.10
1	A	426	CFZ	C4'-O4'-C1'	-3.02	102.79	109.47
1	A	562	UFT	O4-C4-C5	-3.02	119.95	125.16
1	A	288	UFT	O4-C4-C5	-3.02	119.95	125.16
1	A	32	UFT	C3'-C2'-C1'	3.02	106.60	103.10
1	A	17	UFT	O4-C4-C5	-3.01	119.96	125.16
1	A	439	CFZ	C3'-C2'-C1'	3.01	106.60	103.10
1	A	254	UFT	O4-C4-C5	-3.01	119.97	125.16
1	A	657	CFZ	C3'-C2'-C1'	3.01	106.60	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	CFZ	C2'-C3'-C4'	3.01	106.40	102.43
1	A	340	UFT	O4-C4-C5	-3.01	119.97	125.16
1	A	383	UFT	O4-C4-C5	-3.01	119.97	125.16
1	A	6	UFT	O4-C4-C5	-3.01	119.97	125.16
1	A	670	UFT	O4-C4-C5	-3.01	119.98	125.16
1	A	41	CFZ	C3'-C2'-C1'	3.00	106.59	103.10
1	A	590	UFT	O4-C4-C5	-3.00	119.98	125.16
1	A	167	UFT	O4-C4-C5	-3.00	119.98	125.16
1	A	89	UFT	O4-C4-C5	-3.00	119.99	125.16
1	A	644	UFT	O4-C4-C5	-3.00	119.99	125.16
1	A	204	CFZ	C2'-C3'-C4'	3.00	106.39	102.43
1	A	671	UFT	O4-C4-C5	-3.00	119.99	125.16
1	A	541	CFZ	C3'-C2'-C1'	3.00	106.58	103.10
1	A	604	CFZ	C3'-C2'-C1'	3.00	106.58	103.10
1	A	475	UFT	N3-C2-N1	3.00	118.79	114.89
1	A	698	UFT	O4-C4-C5	-3.00	120.00	125.16
1	A	609	CFZ	C2'-C3'-C4'	2.99	106.38	102.43
1	A	388	UFT	O4-C4-C5	-2.99	120.00	125.16
1	A	143	UFT	C3'-C2'-C1'	2.99	106.57	103.10
1	A	123	UFT	O4-C4-C5	-2.99	120.01	125.16
1	A	616	UFT	C3'-C2'-C1'	2.99	106.57	103.10
1	A	397	UFT	C2'-C3'-C4'	2.99	106.37	102.43
1	A	585	UFT	O4-C4-C5	-2.98	120.02	125.16
1	A	642	UFT	O4-C4-C5	-2.98	120.02	125.16
1	A	319	UFT	C2'-C3'-C4'	2.98	106.36	102.43
1	A	192	UFT	O4-C4-C5	-2.98	120.02	125.16
1	A	360	UFT	O4-C4-C5	-2.98	120.03	125.16
1	A	254	UFT	C3'-C2'-C1'	2.98	106.55	103.10
1	A	429	UFT	C2'-C1'-N1	-2.98	109.70	114.27
1	A	156	CFZ	C3'-C2'-C1'	2.97	106.55	103.10
1	A	538	CFZ	C3'-C2'-C1'	2.97	106.55	103.10
1	A	670	UFT	C3'-C2'-C1'	2.97	106.55	103.10
1	A	490	CFZ	C2'-C1'-N1	-2.97	109.71	114.27
1	A	62	UFT	O4-C4-C5	-2.97	120.04	125.16
1	A	196	UFT	O4-C4-C5	-2.97	120.04	125.16
1	A	383	UFT	C2'-C1'-N1	-2.97	109.71	114.27
1	A	558	UFT	C3'-C2'-C1'	2.97	106.54	103.10
1	A	254	UFT	C2'-C1'-N1	-2.97	109.71	114.27
1	A	370	UFT	O4-C4-C5	-2.96	120.05	125.16
1	A	267	UFT	O4-C4-C5	-2.96	120.05	125.16
1	A	148	UFT	O4-C4-C5	-2.96	120.05	125.16
1	A	161	CFZ	C3'-C2'-C1'	2.96	106.54	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	CFZ	C3'-C2'-C1'	2.96	106.54	103.10
1	A	507	UFT	O4-C4-C5	-2.96	120.05	125.16
1	A	538	CFZ	C2'-C1'-N1	-2.96	109.72	114.27
1	A	197	UFT	O4-C4-C5	-2.96	120.06	125.16
1	A	156	CFZ	C2'-C1'-N1	-2.96	109.72	114.27
1	A	588	UFT	O4-C4-C5	-2.96	120.06	125.16
1	A	215	UFT	O4-C4-C5	-2.96	120.06	125.16
1	A	170	UFT	O4-C4-C5	-2.96	120.06	125.16
1	A	563	UFT	O4-C4-C5	-2.96	120.06	125.16
1	A	597	UFT	O4-C4-C5	-2.96	120.06	125.16
1	A	405	CFZ	C2'-C1'-N1	-2.96	109.72	114.27
1	A	128	CFZ	C4'-O4'-C1'	-2.96	102.94	109.47
1	A	88	UFT	O4-C4-C5	-2.96	120.06	125.16
1	A	58	UFT	C3'-C2'-C1'	2.96	106.53	103.10
1	A	476	UFT	O4-C4-C5	-2.95	120.07	125.16
1	A	192	UFT	C3'-C2'-C1'	2.95	106.53	103.10
1	A	142	UFT	O4-C4-C5	-2.95	120.07	125.16
1	A	143	UFT	O4-C4-C5	-2.95	120.07	125.16
1	A	624	UFT	O4-C4-C5	-2.95	120.07	125.16
1	A	421	UFT	O4-C4-C5	-2.95	120.08	125.16
1	A	107	UFT	O4-C4-C5	-2.95	120.08	125.16
1	A	600	CFZ	C2'-C3'-C4'	2.95	106.32	102.43
1	A	104	CFZ	C3'-C2'-C1'	2.95	106.52	103.10
1	A	475	UFT	O4-C4-C5	-2.95	120.08	125.16
1	A	322	UFT	O4-C4-C5	-2.95	120.08	125.16
1	A	585	UFT	C2'-C1'-N1	-2.94	109.75	114.27
1	A	263	UFT	C2'-C3'-C4'	2.94	106.31	102.43
1	A	627	UFT	O4-C4-C5	-2.94	120.09	125.16
1	A	697	UFT	O4-C4-C5	-2.94	120.09	125.16
1	A	693	UFT	C3'-C2'-C1'	2.94	106.51	103.10
1	A	138	UFT	C2'-C1'-N1	-2.94	109.75	114.27
1	A	234	CFZ	C2'-C3'-C4'	2.94	106.30	102.43
1	A	128	CFZ	C2'-C3'-C4'	2.93	106.30	102.43
1	A	162	CFZ	C3'-C2'-C1'	2.93	106.50	103.10
1	A	19	UFT	O4-C4-C5	-2.93	120.11	125.16
1	A	705	UFT	O4-C4-C5	-2.93	120.11	125.16
1	A	181	UFT	C2'-C1'-N1	-2.93	109.77	114.27
1	A	716	UFT	C2'-C3'-C4'	2.93	106.29	102.43
1	A	464	UFT	C2'-C3'-C4'	2.93	106.29	102.43
1	A	103	CFZ	C3'-C2'-C1'	2.93	106.50	103.10
1	A	485	UFT	O4-C4-C5	-2.92	120.12	125.16
1	A	577	CFZ	C2'-C3'-C4'	2.92	106.28	102.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	UFT	O4-C4-C5	-2.92	120.12	125.16
1	A	97	UFT	O4-C4-C5	-2.92	120.12	125.16
1	A	127	UFT	O4-C4-C5	-2.92	120.12	125.16
1	A	549	UFT	O4-C4-C5	-2.92	120.13	125.16
1	A	560	CFZ	C3'-C2'-C1'	2.92	106.49	103.10
1	A	657	CFZ	C2'-C1'-N1	-2.92	109.79	114.27
1	A	617	UFT	O4-C4-C5	-2.92	120.13	125.16
1	A	504	UFT	C2'-C3'-C4'	2.92	106.27	102.43
1	A	589	UFT	O4-C4-C5	-2.91	120.14	125.16
1	A	311	UFT	O4-C4-C5	-2.91	120.14	125.16
1	A	451	UFT	C3'-C2'-C1'	2.91	106.48	103.10
1	A	419	UFT	O4-C4-C5	-2.91	120.14	125.16
1	A	573	UFT	C2'-C3'-C4'	2.91	106.26	102.43
1	A	81	CFZ	C3'-C2'-C1'	2.91	106.47	103.10
1	A	612	UFT	C3'-C2'-C1'	2.90	106.47	103.10
1	A	437	CFZ	C2'-C3'-C4'	2.90	106.26	102.43
1	A	362	CFZ	C4'-O4'-C1'	-2.90	103.06	109.47
1	A	238	UFT	C3'-C2'-C1'	2.90	106.47	103.10
1	A	46	UFT	O4-C4-C5	-2.90	120.16	125.16
1	A	642	UFT	C3'-C2'-C1'	2.90	106.46	103.10
1	A	178	CFZ	C2'-C3'-C4'	2.90	106.25	102.43
1	A	661	CFZ	C2'-C3'-C4'	2.90	106.25	102.43
1	A	564	CFZ	C2'-C3'-C4'	2.90	106.25	102.43
1	A	377	UFT	C4'-O4'-C1'	-2.90	103.07	109.47
1	A	350	UFT	O4-C4-C5	-2.90	120.17	125.16
1	A	345	UFT	C3'-C2'-C1'	2.89	106.46	103.10
1	A	115	UFT	O4-C4-C5	-2.89	120.17	125.16
1	A	144	CFZ	C2'-C3'-C4'	2.89	106.24	102.43
1	A	727	UFT	C2'-C3'-C4'	2.89	106.24	102.43
1	A	351	UFT	O4-C4-C5	-2.89	120.18	125.16
1	A	588	UFT	O2-C2-N1	-2.88	119.05	122.80
1	A	240	UFT	O4-C4-C5	-2.88	120.20	125.16
1	A	416	CFZ	C2'-C3'-C4'	2.88	106.22	102.43
1	A	39	UFT	O4-C4-C5	-2.87	120.20	125.16
1	A	695	CFZ	C2'-C1'-N1	-2.87	109.86	114.27
1	A	616	UFT	O4-C4-C5	-2.87	120.21	125.16
1	A	589	UFT	C3'-C2'-C1'	2.87	106.43	103.10
1	A	12	CFZ	C2'-C3'-C4'	2.87	106.21	102.43
1	A	523	UFT	O4-C4-C5	-2.86	120.23	125.16
1	A	339	UFT	O4-C4-C5	-2.86	120.23	125.16
1	A	483	CFZ	C3'-C2'-C1'	2.86	106.42	103.10
1	A	468	UFT	C2'-C3'-C4'	2.86	106.20	102.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	CFZ	C3'-C2'-C1'	2.86	106.42	103.10
1	A	48	UFT	O4-C4-C5	-2.85	120.24	125.16
1	A	727	UFT	C3'-C2'-C1'	2.85	106.41	103.10
1	A	573	UFT	O4-C4-C5	-2.85	120.24	125.16
1	A	662	UFT	O4-C4-C5	-2.85	120.24	125.16
1	A	556	UFT	O4-C4-C5	-2.85	120.24	125.16
1	A	453	CFZ	C3'-C2'-C1'	2.85	106.41	103.10
1	A	588	UFT	C2'-C1'-N1	-2.85	109.89	114.27
1	A	123	UFT	C2'-C3'-C4'	2.85	106.19	102.43
1	A	33	UFT	C3'-C2'-C1'	2.85	106.41	103.10
1	A	89	UFT	C3'-C2'-C1'	2.84	106.40	103.10
1	A	431	UFT	C2'-C1'-N1	-2.84	109.90	114.27
1	A	33	UFT	C2'-C1'-N1	-2.84	109.90	114.27
1	A	71	UFT	O4-C4-C5	-2.84	120.26	125.16
1	A	61	UFT	C3'-C2'-C1'	2.84	106.40	103.10
1	A	131	CFZ	C2'-C3'-C4'	2.84	106.17	102.43
1	A	550	UFT	C2'-C3'-C4'	2.84	106.17	102.43
1	A	75	CFZ	O2-C2-N3	-2.84	117.86	122.33
1	A	213	UFT	C2'-C3'-C4'	2.84	106.17	102.43
1	A	451	UFT	O4-C4-C5	-2.84	120.27	125.16
1	A	329	UFT	O4-C4-C5	-2.84	120.27	125.16
1	A	693	UFT	C2'-C1'-N1	-2.83	109.92	114.27
1	A	616	UFT	C2'-C3'-C4'	2.83	106.16	102.43
1	A	672	CFZ	C2'-C3'-C4'	2.83	106.16	102.43
1	A	397	UFT	O4-C4-C5	-2.82	120.30	125.16
1	A	719	UFT	O4-C4-C5	-2.82	120.30	125.16
1	A	484	CFZ	C3'-C2'-C1'	2.82	106.37	103.10
1	A	605	CFZ	C3'-C2'-C1'	2.82	106.37	103.10
1	A	206	CFZ	C2'-C3'-C4'	2.81	106.14	102.43
1	A	345	UFT	O4-C4-C5	-2.81	120.31	125.16
1	A	65	CFZ	O2-C2-N3	-2.81	117.90	122.33
1	A	23	UFT	C3'-C2'-C1'	2.81	106.36	103.10
1	A	330	CFZ	C2'-C1'-N1	-2.81	109.96	114.27
1	A	274	UFT	O4-C4-C5	-2.80	120.33	125.16
1	A	575	UFT	O4'-C1'-C2'	-2.80	102.88	105.84
1	A	605	CFZ	C2'-C1'-N1	-2.80	109.97	114.27
1	A	319	UFT	O4-C4-C5	-2.80	120.33	125.16
1	A	644	UFT	C2'-C1'-N1	-2.80	109.97	114.27
1	A	698	UFT	C3'-C2'-C1'	2.80	106.35	103.10
1	A	240	UFT	C2'-C3'-C4'	2.80	106.12	102.43
1	A	283	UFT	C3'-C2'-C1'	2.79	106.34	103.10
1	A	689	CFZ	C3'-C2'-C1'	2.79	106.34	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	UFT	C2'-C1'-N1	-2.79	109.99	114.27
1	A	483	CFZ	C2'-C1'-N1	-2.79	109.99	114.27
1	A	10	CFZ	C3'-C2'-C1'	2.78	106.33	103.10
1	A	689	CFZ	C2'-C1'-N1	-2.78	109.99	114.27
1	A	181	UFT	C5-C4-N3	2.78	118.69	114.80
1	A	532	UFT	C2'-C3'-C4'	2.78	106.09	102.43
1	A	653	CFZ	C2'-C1'-N1	-2.78	110.00	114.27
1	A	197	UFT	C2'-C3'-C4'	2.77	106.09	102.43
1	A	356	UFT	C2'-C3'-C4'	2.77	106.08	102.43
1	A	80	CFZ	C4'-O4'-C1'	-2.77	103.35	109.47
1	A	306	CFZ	C3'-C2'-C1'	2.77	106.31	103.10
1	A	384	CFZ	C3'-C2'-C1'	2.77	106.31	103.10
1	A	242	UFT	C2'-C3'-C4'	2.77	106.08	102.43
1	A	463	CFZ	O2-C2-N3	-2.77	117.97	122.33
1	A	32	UFT	O4-C4-C5	-2.76	120.39	125.16
1	A	87	CFZ	C3'-C2'-C1'	2.76	106.30	103.10
1	A	489	CFZ	C3'-C2'-C1'	2.76	106.30	103.10
1	A	379	CFZ	C2'-C1'-N1	-2.75	110.04	114.27
1	A	208	CFZ	C2'-C3'-C4'	2.75	106.06	102.43
1	A	550	UFT	C3'-C2'-C1'	2.75	106.30	103.10
1	A	79	UFT	O4-C4-C5	-2.75	120.42	125.16
1	A	197	UFT	C2'-C1'-N1	-2.75	110.05	114.27
1	A	366	CFZ	C4'-O4'-C1'	-2.75	103.40	109.47
1	A	291	CFZ	C3'-C2'-C1'	2.75	106.29	103.10
1	A	167	UFT	C2'-C3'-C4'	2.74	106.05	102.43
1	A	607	UFT	O2-C2-N1	-2.74	119.23	122.80
1	A	307	UFT	O4-C4-C5	-2.74	120.43	125.16
1	A	244	CFZ	C3'-C2'-C1'	2.74	106.28	103.10
1	A	602	CFZ	C2'-C3'-C4'	2.74	106.04	102.43
1	A	115	UFT	C3'-C2'-C1'	2.74	106.28	103.10
1	A	193	UFT	C3'-C2'-C1'	2.73	106.27	103.10
1	A	480	UFT	C2'-C1'-N1	-2.73	110.08	114.27
1	A	339	UFT	C1'-N1-C2	2.73	122.49	117.59
1	A	121	CFZ	C3'-C2'-C1'	2.73	106.26	103.10
1	A	366	CFZ	C2'-C1'-N1	-2.72	110.08	114.27
1	A	181	UFT	C2'-C3'-C4'	2.72	106.02	102.43
1	A	417	UFT	C3'-C2'-C1'	2.72	106.26	103.10
1	A	359	CFZ	C1'-N1-C2	2.72	124.45	118.44
1	A	42	UFT	C3'-C2'-C1'	2.72	106.26	103.10
1	A	121	CFZ	C2'-C1'-N1	-2.72	110.09	114.27
1	A	127	UFT	C2'-C1'-N1	-2.72	110.09	114.27
1	A	287	CFZ	C3'-C2'-C1'	2.72	106.25	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	UFT	C2'-C3'-C4'	2.71	106.00	102.43
1	A	269	CFZ	C2'-C3'-C4'	2.71	106.00	102.43
1	A	578	CFZ	O2-C2-N3	-2.71	118.06	122.33
1	A	89	UFT	C2'-C1'-N1	-2.71	110.11	114.27
1	A	194	UFT	C1'-N1-C2	2.71	122.46	117.59
1	A	143	UFT	C2'-C1'-N1	-2.70	110.11	114.27
1	A	562	UFT	C2'-C3'-C4'	2.70	105.99	102.43
1	A	625	CFZ	C3'-C2'-C1'	2.70	106.24	103.10
1	A	713	CFZ	C1'-N1-C2	2.70	124.41	118.44
1	A	422	CFZ	C3'-C2'-C1'	2.70	106.23	103.10
1	A	88	UFT	C2'-C3'-C4'	2.70	105.99	102.43
1	A	456	CFZ	C2'-C3'-C4'	2.70	105.99	102.43
1	A	602	CFZ	C4'-O4'-C1'	-2.70	103.51	109.47
1	A	560	CFZ	C2'-C1'-N1	-2.69	110.13	114.27
1	A	287	CFZ	C2'-C1'-N1	-2.69	110.14	114.27
1	A	154	UFT	O4-C4-C5	-2.69	120.53	125.16
1	A	362	CFZ	C2'-C3'-C4'	2.68	105.97	102.43
1	A	177	UFT	C1'-N1-C2	2.68	122.40	117.59
1	A	727	UFT	O4-C4-C5	-2.68	120.54	125.16
1	A	705	UFT	C2'-C1'-N1	-2.67	110.17	114.27
1	A	272	UFT	O4-C4-C5	-2.66	120.58	125.16
1	A	238	UFT	C2'-C3'-C4'	2.66	105.93	102.43
1	A	346	CFZ	O2-C2-N3	-2.66	118.14	122.33
1	A	332	CFZ	C3'-C2'-C1'	2.66	106.18	103.10
1	A	629	CFZ	O2-C2-N1	2.65	124.10	118.90
1	A	597	UFT	C2'-C1'-N1	-2.65	110.19	114.27
1	A	371	UFT	C3'-C2'-C1'	2.65	106.18	103.10
1	A	151	UFT	O4-C4-C5	-2.65	120.59	125.16
1	A	177	UFT	C2'-C3'-C4'	2.65	105.92	102.43
1	A	563	UFT	C2'-C3'-C4'	2.65	105.92	102.43
1	A	613	CFZ	C2'-C3'-C4'	2.65	105.92	102.43
1	A	643	UFT	C1'-N1-C2	2.65	122.35	117.59
1	A	382	CFZ	C2'-C3'-C4'	2.65	105.92	102.43
1	A	378	CFZ	C2'-C1'-N1	-2.64	110.21	114.27
1	A	409	UFT	C1'-N1-C2	2.64	122.34	117.59
1	A	221	UFT	O4-C4-C5	-2.64	120.61	125.16
1	A	512	CFZ	C2'-C3'-C4'	2.64	105.91	102.43
1	A	432	CFZ	C2'-C3'-C4'	2.64	105.91	102.43
1	A	434	CFZ	C2'-C3'-C4'	2.64	105.91	102.43
1	A	26	CFZ	C2'-C1'-N1	-2.63	110.22	114.27
1	A	329	UFT	C2'-C3'-C4'	2.63	105.90	102.43
1	A	151	UFT	C2'-C1'-N1	-2.63	110.22	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	CFZ	C1'-N1-C2	2.63	124.26	118.44
1	A	377	UFT	O4-C4-C5	-2.63	120.62	125.16
1	A	670	UFT	C2'-C3'-C4'	2.63	105.90	102.43
1	A	638	UFT	C2'-C3'-C4'	2.63	105.89	102.43
1	A	65	CFZ	C2'-C3'-C4'	2.62	105.89	102.43
1	A	359	CFZ	O2-C2-N3	-2.62	118.19	122.33
1	A	93	UFT	C1'-N1-C2	2.62	122.31	117.59
1	A	500	CFZ	C3'-C2'-C1'	2.62	106.14	103.10
1	A	48	UFT	C1'-N1-C2	2.62	122.30	117.59
1	A	562	UFT	C2'-C1'-N1	-2.62	110.24	114.27
1	A	419	UFT	C2'-C3'-C4'	2.62	105.88	102.43
1	A	429	UFT	C1'-N1-C2	2.62	122.30	117.59
1	A	363	CFZ	C2'-C1'-N1	-2.62	110.25	114.27
1	A	563	UFT	C2'-C1'-N1	-2.62	110.25	114.27
1	A	116	UFT	C3'-C2'-C1'	2.61	106.13	103.10
1	A	574	CFZ	C3'-C2'-C1'	2.61	106.13	103.10
1	A	655	UFT	O4-C4-C5	-2.61	120.66	125.16
1	A	244	CFZ	C2'-C1'-N1	-2.61	110.26	114.27
1	A	644	UFT	C3'-C2'-C1'	2.61	106.12	103.10
1	A	80	CFZ	C3'-C2'-C1'	2.60	106.12	103.10
1	A	485	UFT	C2'-C3'-C4'	2.60	105.86	102.43
1	A	480	UFT	O4-C4-C5	-2.60	120.68	125.16
1	A	6	UFT	C2'-C1'-N1	-2.60	110.28	114.27
1	A	162	CFZ	C2'-C3'-C4'	2.60	105.85	102.43
1	A	515	CFZ	O2-C2-N3	-2.59	118.24	122.33
1	A	363	CFZ	C3'-C2'-C1'	2.59	106.11	103.10
1	A	143	UFT	C2'-C3'-C4'	2.59	105.84	102.43
1	A	523	UFT	C2'-C3'-C4'	2.58	105.84	102.43
1	A	686	UFT	O4-C4-C5	-2.57	120.73	125.16
1	A	195	CFZ	C2'-C3'-C4'	2.57	105.81	102.43
1	A	686	UFT	C4'-O4'-C1'	-2.56	103.80	109.47
1	A	328	CFZ	C3'-C2'-C1'	2.56	106.08	103.10
1	A	536	CFZ	F2'-C2'-C3'	2.56	114.20	109.14
1	A	75	CFZ	C1'-N1-C2	2.56	124.09	118.44
1	A	215	UFT	C2'-C3'-C4'	2.56	105.80	102.43
1	A	379	CFZ	O2-C2-N3	-2.56	118.30	122.33
1	A	342	CFZ	C2'-C3'-C4'	2.55	105.80	102.43
1	A	713	CFZ	O2-C2-N3	-2.55	118.30	122.33
1	A	501	UFT	O4-C4-C5	-2.55	120.76	125.16
1	A	444	UFT	C3'-C2'-C1'	2.55	106.06	103.10
1	A	28	CFZ	F2'-C2'-C3'	2.55	114.18	109.14
1	A	687	UFT	C2'-C1'-N1	-2.55	110.36	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	UFT	C2'-C3'-C4'	2.55	105.79	102.43
1	A	624	UFT	C2'-C3'-C4'	2.55	105.79	102.43
1	A	724	UFT	O4-C4-C5	-2.54	120.78	125.16
1	A	161	CFZ	C2'-C1'-N1	-2.54	110.36	114.27
1	A	369	CFZ	C2'-C3'-C4'	2.54	105.78	102.43
1	A	602	CFZ	C2'-C1'-N1	-2.54	110.37	114.27
1	A	151	UFT	C2'-C3'-C4'	2.53	105.77	102.43
1	A	597	UFT	C2'-C3'-C4'	2.53	105.77	102.43
1	A	48	UFT	C3'-C2'-C1'	2.53	106.03	103.10
1	A	83	CFZ	C2'-C1'-N1	-2.52	110.39	114.27
1	A	233	CFZ	C2'-C3'-C4'	2.52	105.76	102.43
1	A	61	UFT	O2-C2-N1	-2.52	119.51	122.80
1	A	419	UFT	C1'-N1-C2	2.52	122.12	117.59
1	A	111	CFZ	C2'-C3'-C4'	2.52	105.75	102.43
1	A	397	UFT	C2'-C1'-N1	-2.52	110.40	114.27
1	A	444	UFT	C2'-C1'-N1	-2.52	110.40	114.27
1	A	196	UFT	C2'-C3'-C4'	2.52	105.75	102.43
1	A	332	CFZ	C2'-C1'-N1	-2.52	110.40	114.27
1	A	26	CFZ	C2'-C3'-C4'	2.52	105.75	102.43
1	A	582	UFT	O4'-C1'-N1	2.51	114.05	108.36
1	A	670	UFT	C2'-C1'-N1	-2.51	110.41	114.27
1	A	346	CFZ	C4'-O4'-C1'	-2.51	103.93	109.47
1	A	709	CFZ	O2-C2-N3	-2.51	118.38	122.33
1	A	56	UFT	C2'-C1'-N1	-2.51	110.42	114.27
1	A	57	CFZ	C2'-C3'-C4'	2.51	105.73	102.43
1	A	374	UFT	O2-C2-N1	-2.51	119.53	122.80
1	A	23	UFT	C1'-N1-C2	2.50	122.09	117.59
1	A	120	UFT	C1'-N1-C2	2.50	122.09	117.59
1	A	429	UFT	O4-C4-C5	-2.50	120.85	125.16
1	A	625	CFZ	C2'-C1'-N1	-2.50	110.43	114.27
1	A	233	CFZ	C2'-C1'-N1	-2.49	110.44	114.27
1	A	308	CFZ	C3'-C2'-C1'	2.49	105.99	103.10
1	A	705	UFT	C3'-C2'-C1'	2.49	105.99	103.10
1	A	706	CFZ	C2'-C1'-N1	-2.49	110.44	114.27
1	A	588	UFT	C2'-C3'-C4'	2.49	105.72	102.43
1	A	578	CFZ	C2'-C3'-C4'	2.49	105.71	102.43
1	A	72	CFZ	C2'-C3'-C4'	2.49	105.71	102.43
1	A	154	UFT	C4'-O4'-C1'	-2.48	103.99	109.47
1	A	487	CFZ	C2'-C1'-N1	-2.48	110.47	114.27
1	A	549	UFT	C2'-C3'-C4'	2.47	105.69	102.43
1	A	728	CFZ	C4'-O4'-C1'	-2.47	104.02	109.47
1	A	322	UFT	O2-C2-N1	-2.47	119.58	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	UFT	C1'-N1-C2	2.46	122.02	117.59
1	A	637	CFZ	C2'-C3'-C4'	2.46	105.68	102.43
1	A	273	CFZ	C2'-C3'-C4'	2.46	105.67	102.43
1	A	697	UFT	C2'-C3'-C4'	2.46	105.67	102.43
1	A	629	CFZ	C1'-N1-C2	2.46	123.87	118.44
1	A	433	CFZ	C2'-C1'-N1	-2.46	110.50	114.27
1	A	6	UFT	C3'-C2'-C1'	2.46	105.95	103.10
1	A	350	UFT	C2'-C3'-C4'	2.45	105.67	102.43
1	A	51	UFT	O2-C2-N1	-2.45	119.60	122.80
1	A	542	UFT	C2'-C1'-N1	-2.45	110.50	114.27
1	A	362	CFZ	O4'-C1'-N1	2.45	113.92	108.36
1	A	632	CFZ	C2'-C3'-C4'	2.45	105.66	102.43
1	A	709	CFZ	C1'-N1-C6	-2.45	115.55	120.78
1	A	307	UFT	C1'-N1-C2	2.45	121.99	117.59
1	A	542	UFT	C2'-C3'-C4'	2.44	105.65	102.43
1	A	330	CFZ	C4'-O4'-C1'	-2.44	104.08	109.47
1	A	167	UFT	C2'-C1'-N1	-2.44	110.53	114.27
1	A	115	UFT	O2-C2-N1	-2.44	119.62	122.80
1	A	493	CFZ	C3'-C2'-C1'	2.43	105.92	103.10
1	A	463	CFZ	C2'-C3'-C4'	2.43	105.64	102.43
1	A	562	UFT	O2-C2-N1	-2.43	119.63	122.80
1	A	464	UFT	C2'-C1'-N1	-2.43	110.54	114.27
1	A	497	UFT	O4-C4-C5	-2.43	120.98	125.16
1	A	575	UFT	O2-C2-N1	-2.42	119.64	122.80
1	A	595	UFT	O2-C2-N1	-2.42	119.64	122.80
1	A	487	CFZ	O2-C2-N3	-2.42	118.51	122.33
1	A	386	CFZ	C4'-O4'-C1'	-2.42	104.12	109.47
1	A	601	UFT	F2'-C2'-C3'	2.42	113.91	109.14
1	A	643	UFT	C3'-C2'-C1'	2.42	105.90	103.10
1	A	188	UFT	C1'-N1-C2	2.41	121.93	117.59
1	A	662	UFT	C4'-O4'-C1'	-2.41	104.14	109.47
1	A	507	UFT	C3'-C2'-C1'	2.41	105.89	103.10
1	A	603	CFZ	O4'-C1'-C2'	2.41	108.39	105.84
1	A	589	UFT	C4'-O4'-C1'	-2.41	104.15	109.47
1	A	444	UFT	O4-C4-C5	-2.40	121.03	125.16
1	A	42	UFT	C2'-C1'-N1	-2.40	110.59	114.27
1	A	371	UFT	O2-C2-N1	-2.40	119.68	122.80
1	A	671	UFT	C1'-N1-C2	2.40	121.89	117.59
1	A	506	CFZ	C2'-C3'-C4'	2.39	105.59	102.43
1	A	360	UFT	C1'-N1-C2	2.39	121.89	117.59
1	A	507	UFT	C2'-C1'-N1	-2.39	110.59	114.27
1	A	632	CFZ	C2'-C1'-N1	-2.39	110.60	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	UFT	C1'-N1-C2	2.39	121.88	117.59
1	A	431	UFT	C2'-C3'-C4'	2.39	105.58	102.43
1	A	351	UFT	C2'-C1'-N1	-2.39	110.60	114.27
1	A	308	CFZ	C2'-C1'-N1	-2.39	110.60	114.27
1	A	467	CFZ	C2'-C1'-N1	-2.38	110.61	114.27
1	A	526	CFZ	O2-C2-N3	-2.38	118.57	122.33
1	A	377	UFT	O4'-C1'-N1	2.38	113.76	108.36
1	A	351	UFT	C2'-C3'-C4'	2.38	105.57	102.43
1	A	575	UFT	C2'-C3'-C4'	2.38	105.57	102.43
1	A	515	CFZ	C1'-N1-C6	-2.38	115.70	120.78
1	A	433	CFZ	C2'-C3'-C4'	2.38	105.56	102.43
1	A	32	UFT	C2'-C3'-C4'	2.38	105.56	102.43
1	A	210	UFT	C1'-N1-C2	2.37	121.86	117.59
1	A	662	UFT	O2-C2-N1	-2.37	119.71	122.80
1	A	291	CFZ	C2'-C3'-C4'	2.37	105.56	102.43
1	A	694	CFZ	C2'-C1'-N1	-2.37	110.63	114.27
1	A	213	UFT	O2-C2-N1	-2.37	119.71	122.80
1	A	109	CFZ	O2-C2-N3	-2.37	118.59	122.33
1	A	510	UFT	O4-C4-C5	-2.37	121.08	125.16
1	A	559	UFT	C2'-C1'-N1	-2.37	110.64	114.27
1	A	188	UFT	O4-C4-C5	-2.36	121.09	125.16
1	A	146	CFZ	C4'-O4'-C1'	-2.36	104.25	109.47
1	A	291	CFZ	C2'-C1'-N1	-2.36	110.64	114.27
1	A	45	CFZ	C2'-C3'-C4'	2.36	105.54	102.43
1	A	138	UFT	C2'-C3'-C4'	2.36	105.54	102.43
1	A	476	UFT	O2-C2-N1	-2.36	119.73	122.80
1	A	154	UFT	C2'-C3'-C4'	2.35	105.53	102.43
1	A	362	CFZ	C2'-C1'-N1	-2.35	110.66	114.27
1	A	131	CFZ	O2-C2-N3	-2.35	118.62	122.33
1	A	198	CFZ	C3'-C2'-C1'	2.35	105.83	103.10
1	A	238	UFT	C2'-C1'-N1	-2.35	110.66	114.27
1	A	15	CFZ	C2'-C1'-N1	-2.35	110.67	114.27
1	A	616	UFT	O2-C2-N1	-2.34	119.75	122.80
1	A	439	CFZ	C2'-C1'-N1	-2.34	110.67	114.27
1	A	686	UFT	O4'-C1'-N1	2.34	113.66	108.36
1	A	213	UFT	C1'-N1-C2	2.34	121.80	117.59
1	A	88	UFT	C2'-C1'-N1	-2.34	110.68	114.27
1	A	370	UFT	C2'-C3'-C4'	2.34	105.51	102.43
1	A	311	UFT	C2'-C1'-N1	-2.34	110.68	114.27
1	A	473	CFZ	F2'-C2'-C3'	2.34	113.75	109.14
1	A	344	CFZ	C2'-C3'-C4'	2.33	105.50	102.43
1	A	169	UFT	C1'-N1-C2	2.33	121.78	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	CFZ	O2-C2-N3	-2.33	118.65	122.33
1	A	661	CFZ	C4'-O4'-C1'	-2.33	104.32	109.47
1	A	244	CFZ	C2'-C3'-C4'	2.33	105.50	102.43
1	A	242	UFT	O2-C2-N1	-2.32	119.77	122.80
1	A	575	UFT	C4'-O4'-C1'	-2.32	104.34	109.47
1	A	367	UFT	O2-C2-N1	-2.32	119.78	122.80
1	A	63	CFZ	C2'-C1'-N1	-2.32	110.71	114.27
1	A	277	UFT	O2-C2-N1	-2.32	119.78	122.80
1	A	62	UFT	C2'-C1'-N1	-2.32	110.71	114.27
1	A	154	UFT	O2-C2-N1	-2.32	119.78	122.80
1	A	490	CFZ	O2-C2-N3	-2.31	118.69	122.33
1	A	311	UFT	O2-C2-N1	-2.31	119.79	122.80
1	A	649	CFZ	C2'-C1'-N1	-2.31	110.72	114.27
1	A	146	CFZ	C2'-C3'-C4'	2.31	105.47	102.43
1	A	283	UFT	O2-C2-N1	-2.31	119.79	122.80
1	A	468	UFT	O4-C4-C5	-2.31	121.19	125.16
1	A	635	CFZ	C2'-C1'-N1	-2.31	110.73	114.27
1	A	48	UFT	C2'-C3'-C4'	2.30	105.47	102.43
1	A	167	UFT	O2-C2-N1	-2.30	119.80	122.80
1	A	61	UFT	C2'-C3'-C4'	2.30	105.46	102.43
1	A	709	CFZ	C2'-C3'-C4'	2.30	105.46	102.43
1	A	490	CFZ	C3'-C2'-C1'	2.30	105.77	103.10
1	A	621	CFZ	O2-C2-N3	-2.30	118.71	122.33
1	A	452	CFZ	C2'-C1'-N1	-2.29	110.75	114.27
1	A	719	UFT	C4'-O4'-C1'	-2.29	104.42	109.47
1	A	641	CFZ	C3'-C2'-C1'	2.28	105.75	103.10
1	A	366	CFZ	O4'-C1'-N1	2.28	113.53	108.36
1	A	577	CFZ	C2'-C1'-N1	-2.28	110.77	114.27
1	A	392	CFZ	C4'-O4'-C1'	-2.28	104.44	109.47
1	A	123	UFT	O2-C2-N1	-2.28	119.83	122.80
1	A	653	CFZ	C3'-C2'-C1'	2.27	105.74	103.10
1	A	361	UFT	O3'-C3'-C2'	2.27	120.21	111.85
1	A	574	CFZ	C4'-O4'-C1'	-2.27	104.45	109.47
1	A	83	CFZ	O2-C2-N3	-2.27	118.75	122.33
1	A	33	UFT	C2'-C3'-C4'	2.27	105.42	102.43
1	A	417	UFT	O4-C4-C5	-2.27	121.25	125.16
1	A	28	CFZ	C5'-C4'-C3'	-2.26	107.06	115.21
1	A	127	UFT	O2-C2-N1	-2.26	119.85	122.80
1	A	650	UFT	C1'-N1-C2	2.26	121.66	117.59
1	A	589	UFT	O2-C2-N1	-2.26	119.86	122.80
1	A	489	CFZ	C2'-C3'-C4'	2.26	105.41	102.43
1	A	686	UFT	O2-C2-N1	-2.26	119.86	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	UFT	O2-C2-N1	-2.26	119.86	122.80
1	A	46	UFT	C2'-C1'-N1	-2.26	110.80	114.27
1	A	621	CFZ	C2'-C3'-C4'	2.26	105.41	102.43
1	A	298	UFT	O4-C4-C5	-2.26	121.27	125.16
1	A	697	UFT	F2'-C2'-C3'	2.26	113.60	109.14
1	A	706	CFZ	F2'-C2'-C3'	2.26	113.60	109.14
1	A	526	CFZ	C1'-N1-C2	2.25	123.42	118.44
1	A	130	CFZ	C2'-C3'-C4'	2.25	105.40	102.43
1	A	662	UFT	C2'-C1'-N1	-2.25	110.81	114.27
1	A	662	UFT	O4'-C1'-N1	2.25	113.46	108.36
1	A	7	CFZ	C4'-O4'-C1'	-2.25	104.50	109.47
1	A	550	UFT	C2'-C1'-N1	-2.25	110.82	114.27
1	A	616	UFT	C2'-C1'-N1	-2.25	110.82	114.27
1	A	157	CFZ	C2'-C3'-C4'	2.25	105.39	102.43
1	A	686	UFT	C2'-C1'-N1	-2.25	110.82	114.27
1	A	656	CFZ	C2'-C1'-N1	-2.25	110.82	114.27
1	A	154	UFT	C2'-C1'-N1	-2.25	110.82	114.27
1	A	104	CFZ	C2'-C3'-C4'	2.24	105.39	102.43
1	A	88	UFT	O2-C2-N1	-2.24	119.88	122.80
1	A	240	UFT	O2-C2-N1	-2.24	119.88	122.80
1	A	66	UFT	C1'-N1-C2	2.24	121.62	117.59
1	A	650	UFT	O2-C2-N1	-2.24	119.88	122.80
1	A	210	UFT	O2-C2-N1	-2.24	119.88	122.80
1	A	683	UFT	O2-C2-N1	-2.24	119.88	122.80
1	A	190	CFZ	C2'-C3'-C4'	2.24	105.38	102.43
1	A	601	UFT	O2-C2-N1	-2.24	119.89	122.80
1	A	497	UFT	C3'-C2'-C1'	2.23	105.69	103.10
1	A	142	UFT	O2-C2-N1	-2.23	119.89	122.80
1	A	667	UFT	O2-C2-N1	-2.23	119.89	122.80
1	A	521	UFT	O4'-C1'-N1	2.23	113.41	108.36
1	A	515	CFZ	N4-C4-N3	2.23	121.89	117.91
1	A	66	UFT	O2-C2-N1	-2.23	119.90	122.80
1	A	303	UFT	O2-C2-N1	-2.22	119.90	122.80
1	A	154	UFT	O4'-C1'-N1	2.22	113.40	108.36
1	A	263	UFT	C2'-C1'-N1	-2.22	110.86	114.27
1	A	148	UFT	C2'-C1'-N1	-2.22	110.86	114.27
1	A	720	CFZ	C4'-O4'-C1'	-2.22	104.56	109.47
1	A	311	UFT	O4'-C1'-N1	2.22	113.39	108.36
1	A	638	UFT	C2'-C1'-N1	-2.21	110.87	114.27
1	A	624	UFT	O2-C2-N1	-2.21	119.92	122.80
1	A	521	UFT	C4'-O4'-C1'	-2.21	104.60	109.47
1	A	521	UFT	O2-C2-N1	-2.20	119.93	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	UFT	O2-C2-N1	-2.20	119.93	122.80
1	A	173	CFZ	C2'-C1'-N1	-2.20	110.89	114.27
1	A	121	CFZ	C4'-O4'-C1'	-2.20	104.61	109.47
1	A	670	UFT	O2-C2-N1	-2.20	119.93	122.80
1	A	182	CFZ	C2'-C1'-N1	-2.20	110.90	114.27
1	A	344	CFZ	C2'-C1'-N1	-2.20	110.90	114.27
1	A	339	UFT	C2'-C3'-C4'	2.20	105.33	102.43
1	A	192	UFT	C2'-C3'-C4'	2.19	105.32	102.43
1	A	175	UFT	F2'-C2'-C3'	2.19	113.47	109.14
1	A	330	CFZ	O2-C2-N3	-2.19	118.88	122.33
1	A	151	UFT	O2-C2-N1	-2.19	119.94	122.80
1	A	638	UFT	O2-C2-N1	-2.19	119.95	122.80
1	A	687	UFT	O2-C2-N1	-2.19	119.95	122.80
1	A	383	UFT	C3'-C2'-C1'	2.19	105.64	103.10
1	A	642	UFT	C2'-C3'-C4'	2.19	105.31	102.43
1	A	550	UFT	C1'-N1-C2	2.18	121.52	117.59
1	A	337	CFZ	C2'-C1'-N1	-2.18	110.92	114.27
1	A	405	CFZ	C4'-O4'-C1'	-2.18	104.65	109.47
1	A	497	UFT	C2'-C3'-C4'	-2.18	99.56	102.43
1	A	663	CFZ	C4'-O4'-C1'	-2.18	104.66	109.47
1	A	361	UFT	O2-C2-N1	-2.18	119.96	122.80
1	A	71	UFT	F2'-C2'-C3'	2.17	113.44	109.14
1	A	57	CFZ	O2-C2-N3	-2.17	118.90	122.33
1	A	39	UFT	C2'-C1'-N1	-2.17	110.93	114.27
1	A	657	CFZ	C4'-O4'-C1'	-2.17	104.68	109.47
1	A	210	UFT	C3'-C2'-C1'	2.17	105.61	103.10
1	A	502	CFZ	C2'-C3'-C4'	2.17	105.28	102.43
1	A	672	CFZ	C3'-C2'-C1'	2.17	105.61	103.10
1	A	196	UFT	O2-C2-N1	-2.17	119.98	122.80
1	A	487	CFZ	C4'-O4'-C1'	-2.16	104.69	109.47
1	A	240	UFT	C2'-C1'-N1	-2.16	110.95	114.27
1	A	89	UFT	O2-C2-N1	-2.16	119.98	122.80
1	A	28	CFZ	C3'-C2'-C1'	2.16	105.61	103.10
1	A	473	CFZ	C2'-C3'-C4'	2.16	105.28	102.43
1	A	340	UFT	O2-C2-N1	-2.16	119.99	122.80
1	A	532	UFT	C2'-C1'-N1	-2.16	110.95	114.27
1	A	107	UFT	O2-C2-N1	-2.16	119.99	122.80
1	A	256	CFZ	C2'-C1'-N1	-2.15	110.96	114.27
1	A	532	UFT	O2-C2-N1	-2.15	119.99	122.80
1	A	397	UFT	O2-C2-N1	-2.15	120.00	122.80
1	A	489	CFZ	C2'-C1'-N1	-2.15	110.97	114.27
1	A	713	CFZ	N4-C4-N3	2.15	121.75	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	UFT	C2'-C3'-C4'	-2.15	99.60	102.43
1	A	103	CFZ	C2'-C3'-C4'	2.15	105.26	102.43
1	A	236	UFT	O2-C2-N1	-2.15	120.00	122.80
1	A	155	CFZ	C2'-C1'-N1	-2.15	110.97	114.27
1	A	173	CFZ	C3'-C2'-C1'	2.14	105.59	103.10
1	A	417	UFT	O4'-C1'-N1	2.14	113.22	108.36
1	A	210	UFT	C2'-C1'-N1	-2.14	110.98	114.27
1	A	698	UFT	O2-C2-N1	-2.14	120.01	122.80
1	A	713	CFZ	C5'-C4'-C3'	-2.14	107.50	115.21
1	A	46	UFT	C3'-C2'-C1'	2.14	105.58	103.10
1	A	374	UFT	C3'-C2'-C1'	2.14	105.58	103.10
1	A	188	UFT	C2'-C3'-C4'	2.14	105.25	102.43
1	A	322	UFT	O4'-C1'-N1	2.14	113.20	108.36
1	A	421	UFT	O2-C2-N1	-2.14	120.01	122.80
1	A	371	UFT	C1'-N1-C2	2.14	121.43	117.59
1	A	62	UFT	O2-C2-N1	-2.14	120.02	122.80
1	A	175	UFT	O3'-C3'-C2'	2.14	119.71	111.85
1	A	311	UFT	C3'-C2'-C1'	2.14	105.58	103.10
1	A	697	UFT	O2-C2-N1	-2.14	120.02	122.80
1	A	111	CFZ	C2'-C1'-N1	-2.13	111.00	114.27
1	A	695	CFZ	C2'-C3'-C4'	2.13	105.24	102.43
1	A	209	CFZ	C2'-C1'-N1	-2.13	111.00	114.27
1	A	138	UFT	O2-C2-N1	-2.13	120.02	122.80
1	A	542	UFT	O2-C2-N1	-2.13	120.03	122.80
1	A	429	UFT	O2-C2-N3	-2.13	117.56	121.49
1	A	559	UFT	O2-C2-N1	-2.13	120.03	122.80
1	A	421	UFT	C3'-C2'-C1'	2.13	105.57	103.10
1	A	148	UFT	C3'-C2'-C1'	2.12	105.57	103.10
1	A	434	CFZ	C3'-C2'-C1'	2.12	105.57	103.10
1	A	129	CFZ	O2-C2-N3	-2.12	118.98	122.33
1	A	345	UFT	O2-C2-N1	-2.12	120.03	122.80
1	A	56	UFT	C1'-N1-C2	2.12	121.40	117.59
1	A	558	UFT	O2-C2-N1	-2.12	120.04	122.80
1	A	644	UFT	O2-C2-N1	-2.12	120.04	122.80
1	A	687	UFT	C3'-C2'-C1'	2.12	105.56	103.10
1	A	563	UFT	O2-C2-N1	-2.11	120.05	122.80
1	A	56	UFT	O2-C2-N1	-2.11	120.05	122.80
1	A	271	CFZ	O2-C2-N3	-2.11	119.00	122.33
1	A	340	UFT	C3'-C2'-C1'	2.11	105.55	103.10
1	A	184	CFZ	C2'-C1'-N1	-2.11	111.03	114.27
1	A	558	UFT	C2'-C1'-N1	-2.11	111.03	114.27
1	A	395	CFZ	C4'-O4'-C1'	-2.11	104.81	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	UFT	C2'-C3'-C4'	2.11	105.21	102.43
1	A	416	CFZ	C1'-N1-C2	2.11	123.09	118.44
1	A	456	CFZ	C2'-C1'-N1	-2.10	111.04	114.27
1	A	17	UFT	F2'-C2'-C3'	2.10	113.30	109.14
1	A	322	UFT	C4'-O4'-C1'	-2.10	104.82	109.47
1	A	328	CFZ	O2-C2-N3	-2.10	119.02	122.33
1	A	32	UFT	O2-C2-N1	-2.10	120.06	122.80
1	A	598	CFZ	C6-C5-C4	2.10	120.97	117.53
1	A	80	CFZ	O4'-C1'-N1	2.10	113.12	108.36
1	A	359	CFZ	C1'-N1-C6	-2.10	116.29	120.78
1	A	582	UFT	O2-C2-N1	-2.10	120.06	122.80
1	A	590	UFT	C2'-C1'-N1	-2.10	111.05	114.27
1	A	658	CFZ	C2'-C1'-N1	-2.09	111.06	114.27
1	A	451	UFT	C2'-C1'-N1	-2.09	111.06	114.27
1	A	221	UFT	C1'-N1-C2	2.09	121.35	117.59
1	A	143	UFT	O2-C2-N1	-2.09	120.08	122.80
1	A	355	CFZ	C2'-C1'-N1	-2.09	111.06	114.27
1	A	407	CFZ	C2'-C1'-N1	-2.09	111.06	114.27
1	A	181	UFT	O4-C4-C5	-2.09	121.56	125.16
1	A	719	UFT	C2'-C3'-C4'	2.09	105.18	102.43
1	A	727	UFT	C1'-N1-C2	2.09	121.34	117.59
1	A	335	CFZ	C1'-N1-C2	2.08	123.04	118.44
1	A	635	CFZ	C2'-C3'-C4'	2.08	105.18	102.43
1	A	468	UFT	C1'-N1-C2	2.08	121.33	117.59
1	A	17	UFT	O3'-C3'-C2'	2.08	119.51	111.85
1	A	466	CFZ	C2'-C3'-C4'	2.08	105.17	102.43
1	A	522	CFZ	C2'-C3'-C4'	2.08	105.17	102.43
1	A	390	UFT	O2-C2-N1	-2.08	120.09	122.80
1	A	28	CFZ	N4-C4-N3	2.08	121.63	117.91
1	A	95	UFT	O2-C2-N1	-2.08	120.09	122.80
1	A	267	UFT	C1'-N1-C2	2.08	121.32	117.59
1	A	193	UFT	O2-C2-N1	-2.07	120.10	122.80
1	A	620	CFZ	C2'-C3'-C4'	2.07	105.16	102.43
1	A	602	CFZ	O4'-C1'-N1	2.07	113.05	108.36
1	A	379	CFZ	C3'-C2'-C1'	2.07	105.50	103.10
1	A	444	UFT	O2-C2-N1	-2.07	120.10	122.80
1	A	536	CFZ	O2-C2-N3	-2.07	119.07	122.33
1	A	212	CFZ	N4-C4-N3	2.07	121.61	117.91
1	A	438	CFZ	O2-C2-N3	-2.07	119.07	122.33
1	A	310	CFZ	C5'-C4'-C3'	-2.07	107.77	115.21
1	A	432	CFZ	O2-C2-N3	-2.07	119.07	122.33
1	A	442	CFZ	O4'-C1'-C2'	2.07	108.03	105.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	UFT	O2-C2-N1	-2.06	120.11	122.80
1	A	135	CFZ	C3'-C2'-C1'	2.06	105.49	103.10
1	A	28	CFZ	O3'-C3'-C2'	2.06	119.43	111.85
1	A	359	CFZ	C5'-C4'-C3'	-2.06	107.79	115.21
1	A	178	CFZ	O2-C2-N3	-2.06	119.08	122.33
1	A	337	CFZ	C3'-C2'-C1'	2.06	105.49	103.10
1	A	590	UFT	O2-C2-N1	-2.06	120.12	122.80
1	A	44	UFT	O2-C2-N1	-2.06	120.12	122.80
1	A	254	UFT	C2'-C3'-C4'	2.06	105.14	102.43
1	A	663	CFZ	O4'-C1'-N1	2.06	113.02	108.36
1	A	343	CFZ	C2'-C3'-C4'	2.05	105.14	102.43
1	A	645	CFZ	O4'-C1'-C2'	2.05	108.02	105.84
1	A	532	UFT	O4-C4-C5	-2.05	121.62	125.16
1	A	727	UFT	F2'-C2'-C3'	2.05	113.19	109.14
1	A	696	CFZ	C3'-C2'-C1'	2.05	105.48	103.10
1	A	55	CFZ	C4'-O4'-C1'	-2.05	104.94	109.47
1	A	335	CFZ	O2-C2-N3	-2.05	119.10	122.33
1	A	170	UFT	C2'-C3'-C4'	2.05	105.13	102.43
1	A	209	CFZ	C2'-C3'-C4'	2.05	105.13	102.43
1	A	557	CFZ	C1'-N1-C2	2.05	122.96	118.44
1	A	405	CFZ	C3'-C2'-C1'	2.04	105.47	103.10
1	A	538	CFZ	O2-C2-N3	-2.04	119.11	122.33
1	A	426	CFZ	C2'-C3'-C4'	2.04	105.12	102.43
1	A	672	CFZ	C4'-O4'-C1'	-2.04	104.96	109.47
1	A	130	CFZ	C2'-C1'-N1	-2.04	111.14	114.27
1	A	549	UFT	C2'-C1'-N1	-2.04	111.14	114.27
1	A	466	CFZ	C4'-O4'-C1'	-2.04	104.97	109.47
1	A	501	UFT	C4'-O4'-C1'	-2.04	104.97	109.47
1	A	655	UFT	C4'-O4'-C1'	-2.03	104.97	109.47
1	A	351	UFT	O2-C2-N1	-2.03	120.15	122.80
1	A	19	UFT	C3'-C2'-C1'	2.03	105.46	103.10
1	A	705	UFT	C2'-C3'-C4'	2.03	105.11	102.43
1	A	497	UFT	O2-C2-N3	-2.03	117.74	121.49
1	A	39	UFT	C3'-C2'-C1'	2.03	105.46	103.10
1	A	555	UFT	C3'-C2'-C1'	2.03	105.46	103.10
1	A	434	CFZ	C5'-C4'-C3'	-2.03	107.91	115.21
1	A	117	CFZ	C2'-C1'-N1	-2.03	111.15	114.27
1	A	263	UFT	O2-C2-N1	-2.03	120.16	122.80
1	A	109	CFZ	C5'-C4'-C3'	-2.03	107.92	115.21
1	A	458	CFZ	C2'-C3'-C4'	2.03	105.10	102.43
1	A	269	CFZ	C2'-C1'-N1	-2.03	111.16	114.27
1	A	34	CFZ	C3'-C2'-C1'	2.02	105.45	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	UFT	C2'-C1'-N1	-2.02	111.16	114.27
1	A	170	UFT	O2-C2-N1	-2.02	120.17	122.80
1	A	208	CFZ	O2-C2-N3	-2.02	119.15	122.33
1	A	41	CFZ	C2'-C3'-C4'	2.01	105.08	102.43
1	A	155	CFZ	C4'-O4'-C1'	-2.01	105.03	109.47
1	A	518	CFZ	C2'-C3'-C4'	2.01	105.08	102.43
1	A	238	UFT	O2-C2-N1	-2.01	120.18	122.80
1	A	439	CFZ	C4'-O4'-C1'	-2.00	105.04	109.47
1	A	501	UFT	O2-C2-N1	-2.00	120.19	122.80
1	A	34	CFZ	O3'-C3'-C2'	2.00	119.22	111.85
1	A	50	CFZ	O4'-C1'-C2'	2.00	107.96	105.84
1	A	458	CFZ	C2'-C1'-N1	-2.00	111.19	114.27
1	A	379	CFZ	N4-C4-N3	2.00	121.49	117.91

There are no chirality outliers.

All (299) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	32	UFT	O4'-C4'-C5'-O5'
1	A	61	UFT	O4'-C4'-C5'-O5'
1	A	62	UFT	O4'-C4'-C5'-O5'
1	A	62	UFT	C3'-C4'-C5'-O5'
1	A	72	CFZ	O4'-C4'-C5'-O5'
1	A	90	CFZ	O4'-C4'-C5'-O5'
1	A	116	UFT	O4'-C4'-C5'-O5'
1	A	128	CFZ	C2'-C1'-N1-C2
1	A	128	CFZ	C2'-C1'-N1-C6
1	A	142	UFT	C4'-C5'-O5'-P
1	A	143	UFT	O4'-C4'-C5'-O5'
1	A	178	CFZ	O4'-C4'-C5'-O5'
1	A	242	UFT	O4'-C4'-C5'-O5'
1	A	242	UFT	C3'-C4'-C5'-O5'
1	A	244	CFZ	O4'-C4'-C5'-O5'
1	A	267	UFT	O4'-C4'-C5'-O5'
1	A	267	UFT	C3'-C4'-C5'-O5'
1	A	345	UFT	O4'-C4'-C5'-O5'
1	A	377	UFT	O4'-C1'-N1-C6
1	A	377	UFT	O4'-C1'-N1-C2
1	A	391	CFZ	C3'-C4'-C5'-O5'
1	A	391	CFZ	O4'-C4'-C5'-O5'
1	A	407	CFZ	C3'-C4'-C5'-O5'
1	A	500	CFZ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	500	CFZ	O4'-C4'-C5'-O5'
1	A	502	CFZ	O4'-C4'-C5'-O5'
1	A	504	UFT	C3'-C4'-C5'-O5'
1	A	515	CFZ	O4'-C4'-C5'-O5'
1	A	522	CFZ	O4'-C4'-C5'-O5'
1	A	526	CFZ	C3'-C4'-C5'-O5'
1	A	526	CFZ	O4'-C4'-C5'-O5'
1	A	550	UFT	C3'-C4'-C5'-O5'
1	A	575	UFT	C2'-C1'-N1-C6
1	A	575	UFT	C2'-C1'-N1-C2
1	A	603	CFZ	C3'-C4'-C5'-O5'
1	A	603	CFZ	O4'-C4'-C5'-O5'
1	A	618	CFZ	O4'-C4'-C5'-O5'
1	A	657	CFZ	C2'-C1'-N1-C2
1	A	657	CFZ	C2'-C1'-N1-C6
1	A	657	CFZ	O4'-C4'-C5'-O5'
1	A	671	UFT	O4'-C1'-N1-C6
1	A	671	UFT	O4'-C1'-N1-C2
1	A	675	CFZ	C3'-C4'-C5'-O5'
1	A	675	CFZ	O4'-C4'-C5'-O5'
1	A	685	CFZ	O4'-C4'-C5'-O5'
1	A	709	CFZ	O4'-C4'-C5'-O5'
1	A	716	UFT	O4'-C4'-C5'-O5'
1	A	719	UFT	O4'-C4'-C5'-O5'
1	A	719	UFT	C3'-C4'-C5'-O5'
1	A	12	CFZ	C3'-C4'-C5'-O5'
1	A	17	UFT	O4'-C4'-C5'-O5'
1	A	17	UFT	C3'-C4'-C5'-O5'
1	A	23	UFT	O4'-C4'-C5'-O5'
1	A	23	UFT	C3'-C4'-C5'-O5'
1	A	32	UFT	C3'-C4'-C5'-O5'
1	A	33	UFT	C3'-C4'-C5'-O5'
1	A	51	UFT	C3'-C4'-C5'-O5'
1	A	61	UFT	C3'-C4'-C5'-O5'
1	A	75	CFZ	O4'-C4'-C5'-O5'
1	A	90	CFZ	C3'-C4'-C5'-O5'
1	A	142	UFT	C3'-C4'-C5'-O5'
1	A	144	CFZ	O4'-C4'-C5'-O5'
1	A	178	CFZ	C3'-C4'-C5'-O5'
1	A	181	UFT	O4'-C4'-C5'-O5'
1	A	198	CFZ	C3'-C4'-C5'-O5'
1	A	198	CFZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	221	UFT	C3'-C4'-C5'-O5'
1	A	244	CFZ	C3'-C4'-C5'-O5'
1	A	271	CFZ	C3'-C4'-C5'-O5'
1	A	291	CFZ	C3'-C4'-C5'-O5'
1	A	291	CFZ	O4'-C4'-C5'-O5'
1	A	330	CFZ	O4'-C4'-C5'-O5'
1	A	360	UFT	O4'-C4'-C5'-O5'
1	A	360	UFT	C3'-C4'-C5'-O5'
1	A	362	CFZ	O4'-C4'-C5'-O5'
1	A	377	UFT	O4'-C4'-C5'-O5'
1	A	377	UFT	C3'-C4'-C5'-O5'
1	A	499	CFZ	C3'-C4'-C5'-O5'
1	A	501	UFT	O4'-C4'-C5'-O5'
1	A	501	UFT	C3'-C4'-C5'-O5'
1	A	502	CFZ	C3'-C4'-C5'-O5'
1	A	515	CFZ	C3'-C4'-C5'-O5'
1	A	527	CFZ	C3'-C4'-C5'-O5'
1	A	588	UFT	C3'-C4'-C5'-O5'
1	A	591	CFZ	C3'-C4'-C5'-O5'
1	A	591	CFZ	O4'-C4'-C5'-O5'
1	A	644	UFT	O4'-C4'-C5'-O5'
1	A	658	CFZ	C3'-C4'-C5'-O5'
1	A	685	CFZ	C3'-C4'-C5'-O5'
1	A	696	CFZ	C3'-C4'-C5'-O5'
1	A	709	CFZ	C3'-C4'-C5'-O5'
1	A	716	UFT	C3'-C4'-C5'-O5'
1	A	206	CFZ	C4'-C5'-O5'-P
1	A	303	UFT	C4'-C5'-O5'-P
1	A	595	UFT	C4'-C5'-O5'-P
1	A	55	CFZ	O4'-C4'-C5'-O5'
1	A	72	CFZ	C3'-C4'-C5'-O5'
1	A	144	CFZ	C3'-C4'-C5'-O5'
1	A	221	UFT	O4'-C4'-C5'-O5'
1	A	271	CFZ	O4'-C4'-C5'-O5'
1	A	274	UFT	O4'-C4'-C5'-O5'
1	A	274	UFT	C3'-C4'-C5'-O5'
1	A	359	CFZ	O4'-C4'-C5'-O5'
1	A	366	CFZ	C3'-C4'-C5'-O5'
1	A	407	CFZ	O4'-C4'-C5'-O5'
1	A	468	UFT	C3'-C4'-C5'-O5'
1	A	475	UFT	O4'-C4'-C5'-O5'
1	A	475	UFT	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	499	CFZ	O4'-C4'-C5'-O5'
1	A	504	UFT	O4'-C4'-C5'-O5'
1	A	550	UFT	O4'-C4'-C5'-O5'
1	A	588	UFT	O4'-C4'-C5'-O5'
1	A	589	UFT	C3'-C4'-C5'-O5'
1	A	617	UFT	O4'-C4'-C5'-O5'
1	A	713	CFZ	C3'-C4'-C5'-O5'
1	A	713	CFZ	O4'-C4'-C5'-O5'
1	A	728	CFZ	C3'-C4'-C5'-O5'
1	A	728	CFZ	O4'-C4'-C5'-O5'
1	A	171	CFZ	C3'-C4'-C5'-O5'
1	A	345	UFT	C3'-C4'-C5'-O5'
1	A	359	CFZ	C3'-C4'-C5'-O5'
1	A	522	CFZ	C3'-C4'-C5'-O5'
1	A	618	CFZ	C3'-C4'-C5'-O5'
1	A	657	CFZ	C3'-C4'-C5'-O5'
1	A	120	UFT	C4'-C5'-O5'-P
1	A	188	UFT	C4'-C5'-O5'-P
1	A	409	UFT	C4'-C5'-O5'-P
1	A	501	UFT	C4'-C5'-O5'-P
1	A	589	UFT	C4'-C5'-O5'-P
1	A	57	CFZ	C3'-C4'-C5'-O5'
1	A	116	UFT	C3'-C4'-C5'-O5'
1	A	143	UFT	C3'-C4'-C5'-O5'
1	A	438	CFZ	C3'-C4'-C5'-O5'
1	A	564	CFZ	C3'-C4'-C5'-O5'
1	A	631	CFZ	C3'-C4'-C5'-O5'
1	A	655	UFT	C3'-C4'-C5'-O5'
1	A	658	CFZ	O4'-C4'-C5'-O5'
1	A	683	UFT	O4'-C4'-C5'-O5'
1	A	307	UFT	C4'-C5'-O5'-P
1	A	12	CFZ	O4'-C4'-C5'-O5'
1	A	33	UFT	O4'-C4'-C5'-O5'
1	A	51	UFT	O4'-C4'-C5'-O5'
1	A	71	UFT	C3'-C4'-C5'-O5'
1	A	75	CFZ	C3'-C4'-C5'-O5'
1	A	94	UFT	C3'-C4'-C5'-O5'
1	A	330	CFZ	C3'-C4'-C5'-O5'
1	A	362	CFZ	C3'-C4'-C5'-O5'
1	A	366	CFZ	O4'-C4'-C5'-O5'
1	A	367	UFT	O4'-C4'-C5'-O5'
1	A	527	CFZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	585	UFT	O4'-C4'-C5'-O5'
1	A	589	UFT	O4'-C4'-C5'-O5'
1	A	644	UFT	C3'-C4'-C5'-O5'
1	A	661	CFZ	O4'-C4'-C5'-O5'
1	A	696	CFZ	O4'-C4'-C5'-O5'
1	A	115	UFT	C4'-C5'-O5'-P
1	A	177	UFT	C4'-C5'-O5'-P
1	A	208	CFZ	C4'-C5'-O5'-P
1	A	346	CFZ	C4'-C5'-O5'-P
1	A	115	UFT	C3'-C4'-C5'-O5'
1	A	142	UFT	O4'-C4'-C5'-O5'
1	A	643	UFT	C3'-C4'-C5'-O5'
1	A	661	CFZ	C3'-C4'-C5'-O5'
1	A	674	CFZ	C4'-C5'-O5'-P
1	A	719	UFT	C4'-C5'-O5'-P
1	A	57	CFZ	O4'-C4'-C5'-O5'
1	A	564	CFZ	O4'-C4'-C5'-O5'
1	A	672	CFZ	C3'-C4'-C5'-O5'
1	A	62	UFT	C4'-C5'-O5'-P
1	A	94	UFT	C4'-C5'-O5'-P
1	A	196	UFT	C4'-C5'-O5'-P
1	A	359	CFZ	C4'-C5'-O5'-P
1	A	360	UFT	C4'-C5'-O5'-P
1	A	512	CFZ	C4'-C5'-O5'-P
1	A	642	UFT	C4'-C5'-O5'-P
1	A	685	CFZ	C4'-C5'-O5'-P
1	A	713	CFZ	C4'-C5'-O5'-P
1	A	71	UFT	O4'-C4'-C5'-O5'
1	A	181	UFT	C3'-C4'-C5'-O5'
1	A	329	UFT	O4'-C4'-C5'-O5'
1	A	468	UFT	O4'-C4'-C5'-O5'
1	A	650	UFT	O4'-C4'-C5'-O5'
1	A	655	UFT	O4'-C4'-C5'-O5'
1	A	94	UFT	O4'-C4'-C5'-O5'
1	A	128	CFZ	O4'-C4'-C5'-O5'
1	A	438	CFZ	O4'-C4'-C5'-O5'
1	A	274	UFT	C4'-C5'-O5'-P
1	A	475	UFT	C4'-C5'-O5'-P
1	A	322	UFT	O4'-C4'-C5'-O5'
1	A	490	CFZ	C3'-C4'-C5'-O5'
1	A	631	CFZ	O4'-C4'-C5'-O5'
1	A	674	CFZ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	683	UFT	C3'-C4'-C5'-O5'
1	A	128	CFZ	C3'-C4'-C5'-O5'
1	A	322	UFT	C3'-C4'-C5'-O5'
1	A	476	UFT	O4'-C4'-C5'-O5'
1	A	476	UFT	C3'-C4'-C5'-O5'
1	A	670	UFT	C3'-C4'-C5'-O5'
1	A	643	UFT	O4'-C1'-N1-C6
1	A	727	UFT	C4'-C5'-O5'-P
1	A	728	CFZ	C2'-C1'-N1-C2
1	A	728	CFZ	C2'-C1'-N1-C6
1	A	575	UFT	O4'-C1'-N1-C6
1	A	88	UFT	C3'-C4'-C5'-O5'
1	A	114	CFZ	C3'-C4'-C5'-O5'
1	A	617	UFT	C3'-C4'-C5'-O5'
1	A	643	UFT	O4'-C1'-N1-C2
1	A	146	CFZ	C4'-C5'-O5'-P
1	A	128	CFZ	O4'-C1'-N1-C6
1	A	44	UFT	O4'-C4'-C5'-O5'
1	A	73	CFZ	C3'-C4'-C5'-O5'
1	A	154	UFT	O4'-C4'-C5'-O5'
1	A	273	CFZ	O4'-C4'-C5'-O5'
1	A	371	UFT	C3'-C4'-C5'-O5'
1	A	521	UFT	C3'-C4'-C5'-O5'
1	A	531	CFZ	O4'-C4'-C5'-O5'
1	A	645	CFZ	C3'-C4'-C5'-O5'
1	A	674	CFZ	O4'-C4'-C5'-O5'
1	A	724	UFT	O4'-C4'-C5'-O5'
1	A	575	UFT	O4'-C1'-N1-C2
1	A	88	UFT	C4'-C5'-O5'-P
1	A	131	CFZ	C4'-C5'-O5'-P
1	A	578	CFZ	C4'-C5'-O5'-P
1	A	621	CFZ	C4'-C5'-O5'-P
1	A	644	UFT	C4'-C5'-O5'-P
1	A	670	UFT	C4'-C5'-O5'-P
1	A	57	CFZ	C4'-C5'-O5'-P
1	A	335	CFZ	C4'-C5'-O5'-P
1	A	438	CFZ	C4'-C5'-O5'-P
1	A	490	CFZ	C4'-C5'-O5'-P
1	A	502	CFZ	C4'-C5'-O5'-P
1	A	605	CFZ	C4'-C5'-O5'-P
1	A	675	CFZ	C4'-C5'-O5'-P
1	A	34	CFZ	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	39	UFT	C3'-C4'-C5'-O5'
1	A	55	CFZ	C3'-C4'-C5'-O5'
1	A	208	CFZ	C3'-C4'-C5'-O5'
1	A	382	CFZ	C3'-C4'-C5'-O5'
1	A	585	UFT	C3'-C4'-C5'-O5'
1	A	649	CFZ	C3'-C4'-C5'-O5'
1	A	271	CFZ	C4'-C5'-O5'-P
1	A	377	UFT	C4'-C5'-O5'-P
1	A	697	UFT	C4'-C5'-O5'-P
1	A	171	CFZ	O4'-C4'-C5'-O5'
1	A	71	UFT	C4'-C5'-O5'-P
1	A	617	UFT	C4'-C5'-O5'-P
1	A	643	UFT	O4'-C4'-C5'-O5'
1	A	657	CFZ	O4'-C1'-N1-C6
1	A	616	UFT	C4'-C5'-O5'-P
1	A	709	CFZ	C4'-C5'-O5'-P
1	A	573	UFT	C4'-C5'-O5'-P
1	A	115	UFT	O4'-C4'-C5'-O5'
1	A	182	CFZ	O4'-C4'-C5'-O5'
1	A	397	UFT	O4'-C4'-C5'-O5'
1	A	490	CFZ	O4'-C4'-C5'-O5'
1	A	510	UFT	O4'-C4'-C5'-O5'
1	A	521	UFT	O4'-C4'-C5'-O5'
1	A	526	CFZ	C4'-C5'-O5'-P
1	A	728	CFZ	C4'-C5'-O5'-P
1	A	371	UFT	O4'-C4'-C5'-O5'
1	A	531	CFZ	C3'-C4'-C5'-O5'
1	A	649	CFZ	O4'-C4'-C5'-O5'
1	A	128	CFZ	O4'-C1'-N1-C2
1	A	208	CFZ	O4'-C4'-C5'-O5'
1	A	590	UFT	O4'-C4'-C5'-O5'
1	A	645	CFZ	O4'-C4'-C5'-O5'
1	A	6	UFT	C3'-C4'-C5'-O5'
1	A	217	CFZ	C3'-C4'-C5'-O5'
1	A	256	CFZ	O4'-C4'-C5'-O5'
1	A	221	UFT	C4'-C5'-O5'-P
1	A	607	UFT	C3'-C4'-C5'-O5'
1	A	500	CFZ	C4'-C5'-O5'-P
1	A	590	UFT	C4'-C5'-O5'-P
1	A	658	CFZ	C4'-C5'-O5'-P
1	A	72	CFZ	C2'-C1'-N1-C2
1	A	72	CFZ	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	A	377	UFT	C2'-C1'-N1-C2
1	A	460	CFZ	C2'-C1'-N1-C2
1	A	476	UFT	C2'-C1'-N1-C2
1	A	573	UFT	C2'-C1'-N1-C6
1	A	602	CFZ	C2'-C1'-N1-C2
1	A	602	CFZ	C2'-C1'-N1-C6
1	A	709	CFZ	C2'-C1'-N1-C6
1	A	34	CFZ	O4'-C4'-C5'-O5'
1	A	88	UFT	O4'-C4'-C5'-O5'
1	A	336	CFZ	C3'-C4'-C5'-O5'
1	A	382	CFZ	O4'-C4'-C5'-O5'
1	A	557	CFZ	C3'-C4'-C5'-O5'
1	A	650	UFT	C3'-C4'-C5'-O5'
1	A	657	CFZ	O4'-C1'-N1-C2
1	A	329	UFT	C3'-C4'-C5'-O5'
1	A	367	UFT	C3'-C4'-C5'-O5'
1	A	128	CFZ	C4'-C5'-O5'-P
1	A	178	CFZ	C4'-C5'-O5'-P
1	A	504	UFT	C4'-C5'-O5'-P
1	A	591	CFZ	C4'-C5'-O5'-P
1	A	607	UFT	C4'-C5'-O5'-P
1	A	655	UFT	C4'-C5'-O5'-P
1	A	114	CFZ	O4'-C4'-C5'-O5'

There are no ring outliers.

279 monomers are involved in 430 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	161	CFZ	1	0
1	A	11	CFZ	2	0
1	A	485	UFT	2	0
1	A	426	CFZ	1	0
1	A	542	UFT	2	0
1	A	661	CFZ	1	0
1	A	627	UFT	1	0
1	A	346	CFZ	1	0
1	A	128	CFZ	1	0
1	A	236	UFT	2	0
1	A	658	CFZ	1	0
1	A	206	CFZ	2	0
1	A	275	CFZ	4	0
1	A	51	UFT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	577	CFZ	1	0
1	A	95	UFT	2	0
1	A	283	UFT	3	0
1	A	518	CFZ	2	0
1	A	471	UFT	4	0
1	A	329	UFT	1	0
1	A	45	CFZ	3	0
1	A	687	UFT	3	0
1	A	72	CFZ	2	0
1	A	675	CFZ	1	0
1	A	175	UFT	3	0
1	A	475	UFT	1	0
1	A	667	UFT	2	0
1	A	50	CFZ	1	0
1	A	585	UFT	2	0
1	A	165	CFZ	3	0
1	A	56	UFT	1	0
1	A	433	CFZ	1	0
1	A	575	UFT	2	0
1	A	444	UFT	2	0
1	A	650	UFT	3	0
1	A	602	CFZ	1	0
1	A	683	UFT	1	0
1	A	137	CFZ	2	0
1	A	500	CFZ	2	0
1	A	416	CFZ	3	0
1	A	607	UFT	3	0
1	A	101	CFZ	1	0
1	A	184	CFZ	1	0
1	A	460	CFZ	2	0
1	A	233	CFZ	1	0
1	A	355	CFZ	2	0
1	A	442	CFZ	1	0
1	A	193	UFT	2	0
1	A	308	CFZ	1	0
1	A	609	CFZ	3	0
1	A	311	UFT	2	0
1	A	649	CFZ	3	0
1	A	337	CFZ	3	0
1	A	618	CFZ	1	0
1	A	727	UFT	1	0
1	A	392	CFZ	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	274	UFT	3	0
1	A	637	CFZ	2	0
1	A	93	UFT	2	0
1	A	154	UFT	2	0
1	A	215	UFT	4	0
1	A	382	CFZ	3	0
1	A	162	CFZ	1	0
1	A	129	CFZ	3	0
1	A	111	CFZ	3	0
1	A	556	UFT	1	0
1	A	138	UFT	1	0
1	A	332	CFZ	3	0
1	A	391	CFZ	2	0
1	A	724	UFT	3	0
1	A	153	CFZ	1	0
1	A	48	UFT	2	0
1	A	483	CFZ	1	0
1	A	438	CFZ	2	0
1	A	388	UFT	1	0
1	A	360	UFT	2	0
1	A	123	UFT	1	0
1	A	208	CFZ	2	0
1	A	451	UFT	2	0
1	A	439	CFZ	3	0
1	A	690	CFZ	1	0
1	A	121	CFZ	3	0
1	A	345	UFT	2	0
1	A	108	CFZ	1	0
1	A	456	CFZ	2	0
1	A	417	UFT	4	0
1	A	330	CFZ	4	0
1	A	361	UFT	2	0
1	A	350	UFT	2	0
1	A	319	UFT	2	0
1	A	502	CFZ	2	0
1	A	573	UFT	1	0
1	A	625	CFZ	4	0
1	A	240	UFT	1	0
1	A	466	CFZ	1	0
1	A	603	CFZ	1	0
1	A	555	UFT	1	0
1	A	190	CFZ	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	384	CFZ	1	0
1	A	452	CFZ	3	0
1	A	657	CFZ	2	0
1	A	473	CFZ	1	0
1	A	612	UFT	2	0
1	A	674	CFZ	1	0
1	A	103	CFZ	3	0
1	A	557	CFZ	1	0
1	A	307	UFT	2	0
1	A	273	CFZ	3	0
1	A	532	UFT	1	0
1	A	497	UFT	1	0
1	A	538	CFZ	2	0
1	A	601	UFT	1	0
1	A	28	CFZ	3	0
1	A	629	CFZ	1	0
1	A	695	CFZ	1	0
1	A	177	UFT	2	0
1	A	23	UFT	2	0
1	A	209	CFZ	3	0
1	A	156	CFZ	1	0
1	A	170	UFT	1	0
1	A	104	CFZ	2	0
1	A	397	UFT	1	0
1	A	510	UFT	1	0
1	A	594	CFZ	3	0
1	A	419	UFT	3	0
1	A	335	CFZ	2	0
1	A	685	CFZ	1	0
1	A	12	CFZ	3	0
1	A	306	CFZ	3	0
1	A	39	UFT	2	0
1	A	363	CFZ	2	0
1	A	467	CFZ	1	0
1	A	366	CFZ	3	0
1	A	263	UFT	1	0
1	A	310	CFZ	1	0
1	A	476	UFT	1	0
1	A	272	UFT	2	0
1	A	157	CFZ	2	0
1	A	7	CFZ	3	0
1	A	597	UFT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	521	UFT	5	0
1	A	351	UFT	3	0
1	A	487	CFZ	3	0
1	A	598	CFZ	1	0
1	A	212	CFZ	2	0
1	A	155	CFZ	1	0
1	A	480	UFT	1	0
1	A	242	UFT	1	0
1	A	531	CFZ	2	0
1	A	662	UFT	3	0
1	A	302	CFZ	3	0
1	A	26	CFZ	1	0
1	A	377	UFT	5	0
1	A	234	CFZ	4	0
1	A	343	CFZ	4	0
1	A	356	UFT	2	0
1	A	574	CFZ	2	0
1	A	130	CFZ	2	0
1	A	432	CFZ	1	0
1	A	421	UFT	2	0
1	A	666	CFZ	4	0
1	A	117	CFZ	1	0
1	A	367	UFT	3	0
1	A	437	CFZ	2	0
1	A	66	UFT	2	0
1	A	109	CFZ	2	0
1	A	210	UFT	2	0
1	A	288	UFT	1	0
1	A	489	CFZ	1	0
1	A	512	CFZ	2	0
1	A	453	CFZ	4	0
1	A	219	CFZ	3	0
1	A	107	UFT	2	0
1	A	271	CFZ	1	0
1	A	407	CFZ	3	0
1	A	665	CFZ	2	0
1	A	44	UFT	3	0
1	A	643	UFT	1	0
1	A	484	CFZ	1	0
1	A	314	CFZ	1	0
1	A	559	UFT	2	0
1	A	147	CFZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	80	CFZ	1	0
1	A	55	CFZ	3	0
1	A	617	UFT	1	0
1	A	46	UFT	3	0
1	A	41	CFZ	2	0
1	A	504	UFT	2	0
1	A	254	UFT	1	0
1	A	374	UFT	1	0
1	A	522	CFZ	4	0
1	A	620	CFZ	2	0
1	A	79	UFT	1	0
1	A	541	CFZ	3	0
1	A	527	CFZ	1	0
1	A	71	UFT	1	0
1	A	276	CFZ	3	0
1	A	507	UFT	1	0
1	A	244	CFZ	2	0
1	A	582	UFT	4	0
1	A	217	CFZ	4	0
1	A	342	CFZ	3	0
1	A	33	UFT	1	0
1	A	624	UFT	2	0
1	A	94	UFT	3	0
1	A	468	UFT	3	0
1	A	178	CFZ	2	0
1	A	34	CFZ	2	0
1	A	204	CFZ	2	0
1	A	287	CFZ	2	0
1	A	359	CFZ	1	0
1	A	613	CFZ	3	0
1	A	213	UFT	3	0
1	A	713	CFZ	4	0
1	A	390	UFT	1	0
1	A	705	UFT	2	0
1	A	340	UFT	5	0
1	A	192	UFT	3	0
1	A	536	CFZ	2	0
1	A	561	CFZ	1	0
1	A	693	UFT	1	0
1	A	383	UFT	3	0
1	A	97	UFT	3	0
1	A	591	CFZ	1	0

*Continued on next page...*



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	344	CFZ	2	0
1	A	188	UFT	3	0
1	A	589	UFT	1	0
1	A	114	CFZ	1	0
1	A	501	UFT	1	0
1	A	422	CFZ	3	0
1	A	32	UFT	1	0
1	A	291	CFZ	1	0
1	A	547	CFZ	2	0
1	A	490	CFZ	2	0
1	A	653	CFZ	2	0
1	A	499	CFZ	1	0
1	A	523	UFT	2	0
1	A	171	CFZ	2	0
1	A	267	UFT	2	0
1	A	256	CFZ	3	0
1	A	493	CFZ	1	0
1	A	173	CFZ	3	0
1	A	616	UFT	1	0
1	A	663	CFZ	3	0
1	A	638	UFT	2	0
1	A	549	UFT	2	0
1	A	135	CFZ	2	0
1	A	689	CFZ	2	0
1	A	81	CFZ	1	0
1	A	339	UFT	3	0
1	A	635	CFZ	3	0
1	A	120	UFT	1	0
1	A	322	UFT	1	0
1	A	429	UFT	1	0
1	A	431	UFT	1	0
1	A	694	CFZ	2	0
1	A	362	CFZ	1	0
1	A	558	UFT	2	0
1	A	716	UFT	1	0
1	A	686	UFT	2	0
1	A	458	CFZ	2	0
1	A	706	CFZ	4	0
1	A	42	UFT	3	0
1	A	19	UFT	1	0
1	A	336	CFZ	3	0
1	A	588	UFT	2	0

*Continued on next page...*



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	146	CFZ	1	0
1	A	277	UFT	2	0
1	A	303	UFT	2	0
1	A	148	UFT	3	0
1	A	230	UFT	2	0
1	A	560	CFZ	2	0
1	A	73	CFZ	1	0
1	A	83	CFZ	3	0
1	A	546	CFZ	2	0
1	A	550	UFT	3	0
1	A	10	CFZ	2	0
1	A	6	UFT	1	0
1	A	131	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.



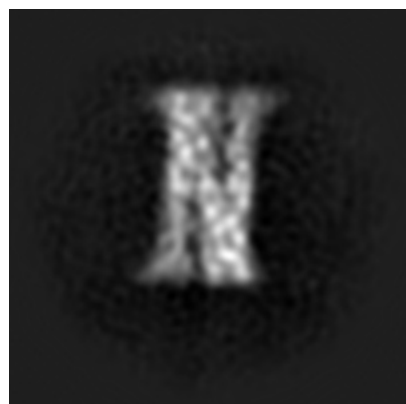
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53803. These allow visual inspection of the internal detail of the map and identification of artifacts.

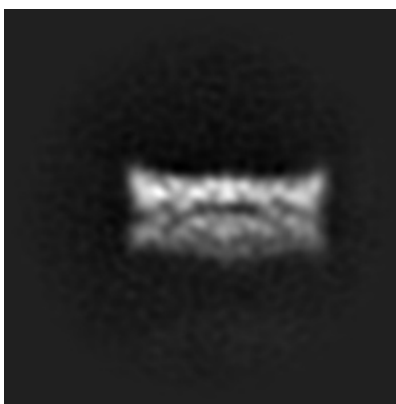
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X

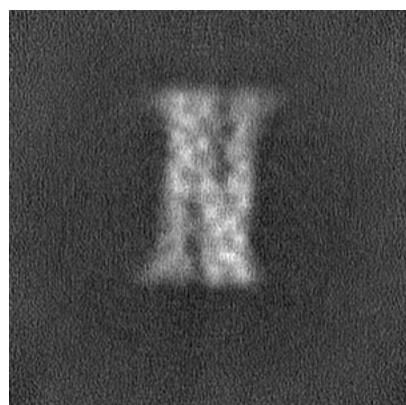


Y

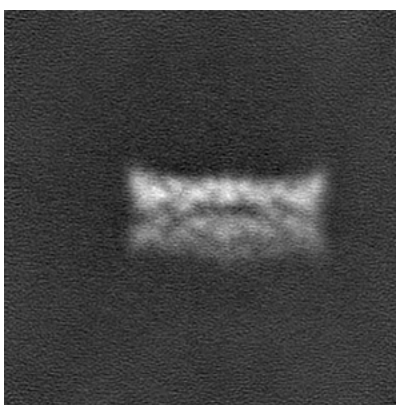


Z

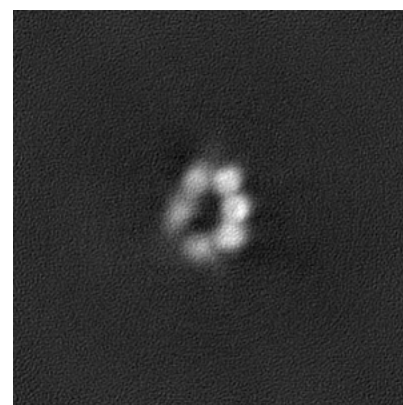
#### 6.1.2 Raw map



X



Y



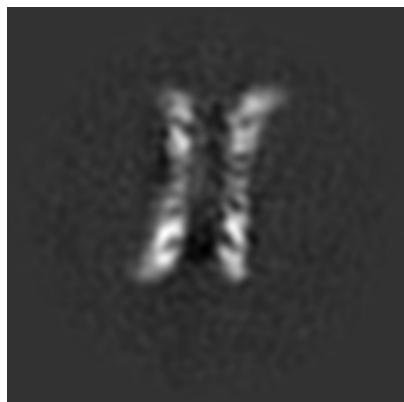
Z

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



## 6.2 Central slices [i](#)

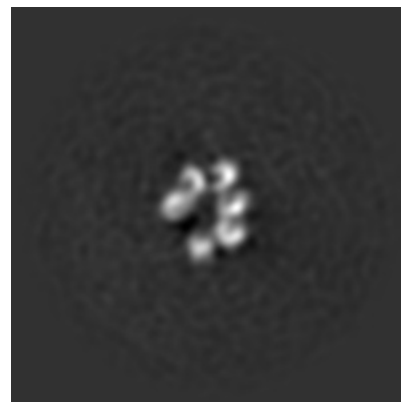
### 6.2.1 Primary map



X Index: 128

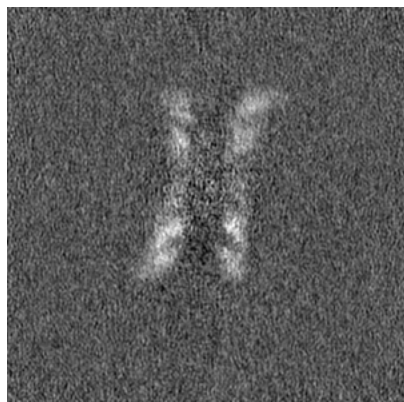


Y Index: 128

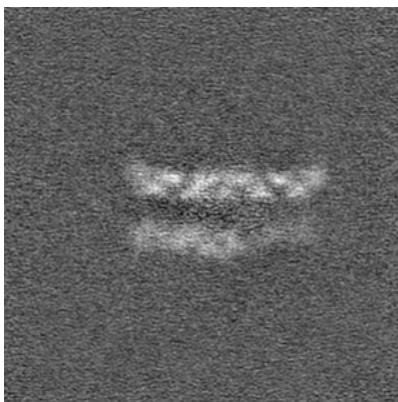


Z Index: 128

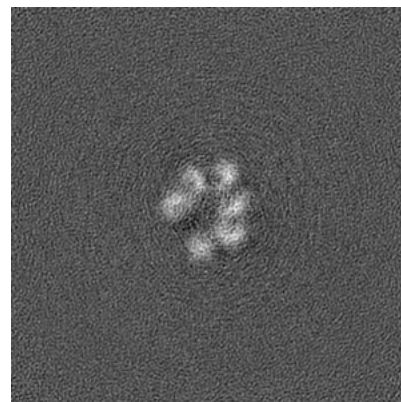
### 6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

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

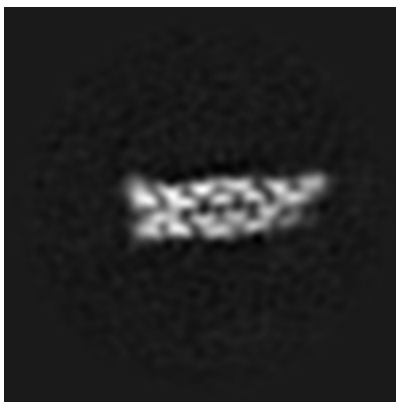


## 6.3 Largest variance slices [i](#)

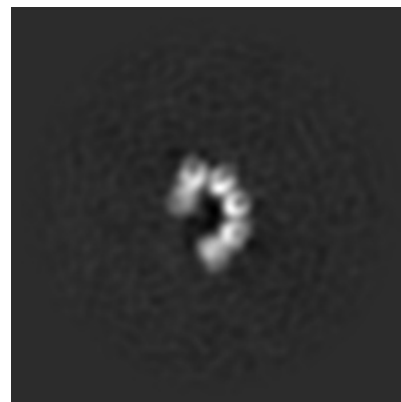
### 6.3.1 Primary map



X Index: 139

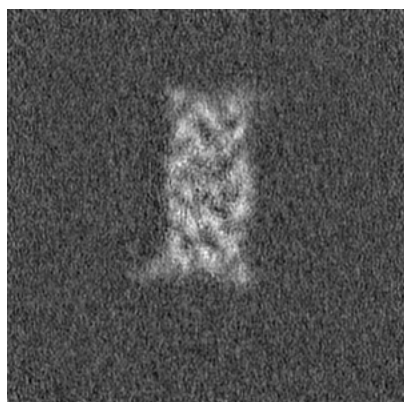


Y Index: 147

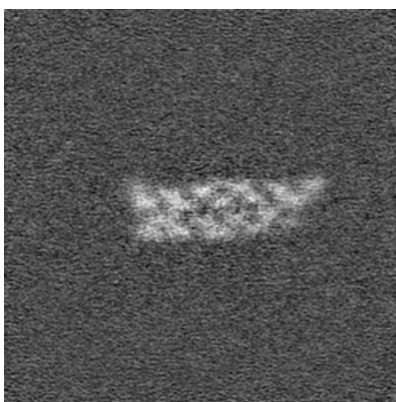


Z Index: 97

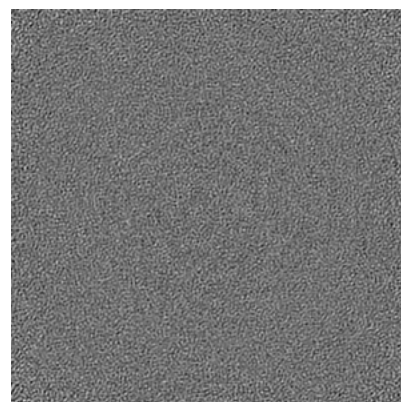
### 6.3.2 Raw map



X Index: 139



Y Index: 147



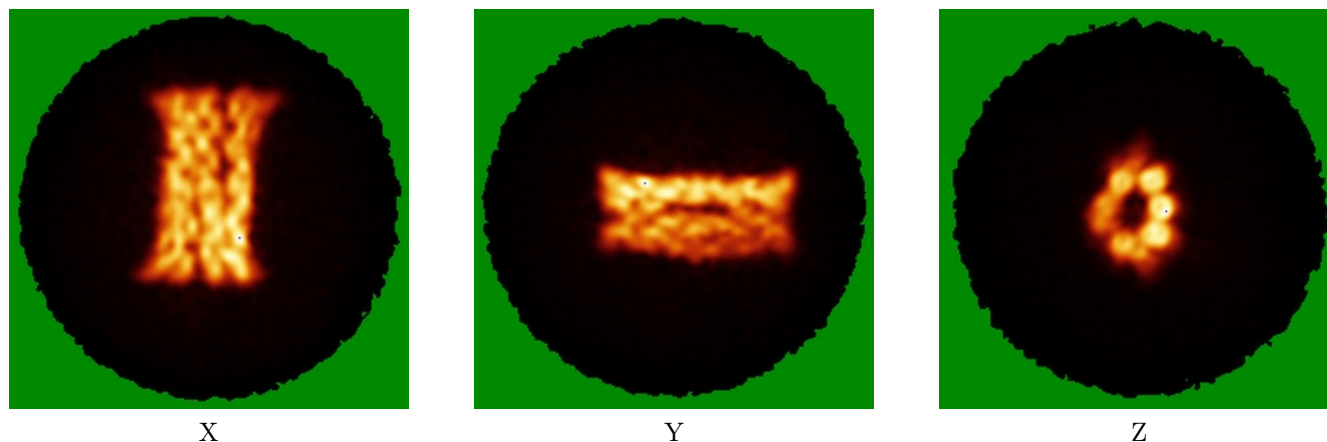
Z Index: 0

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

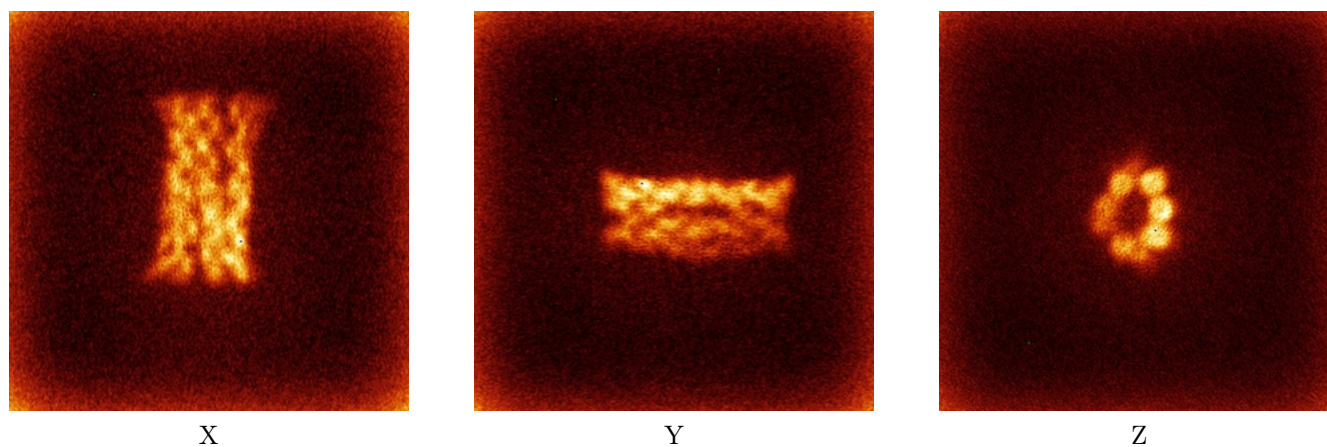


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map

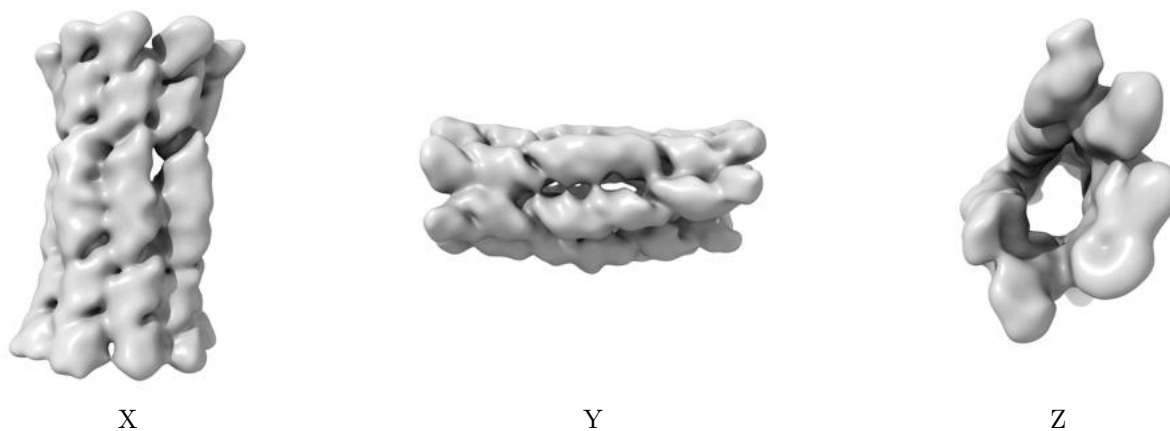


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



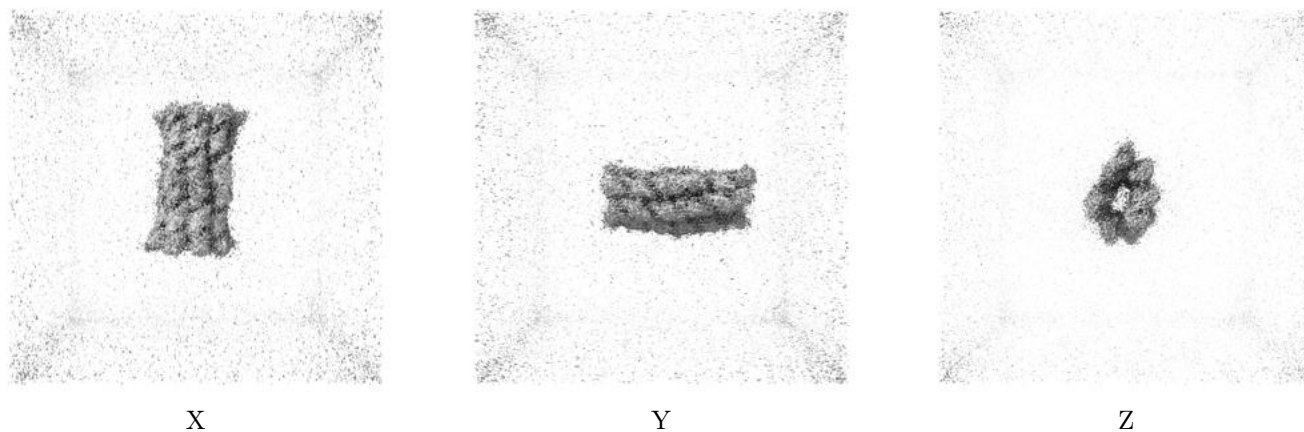
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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](#)

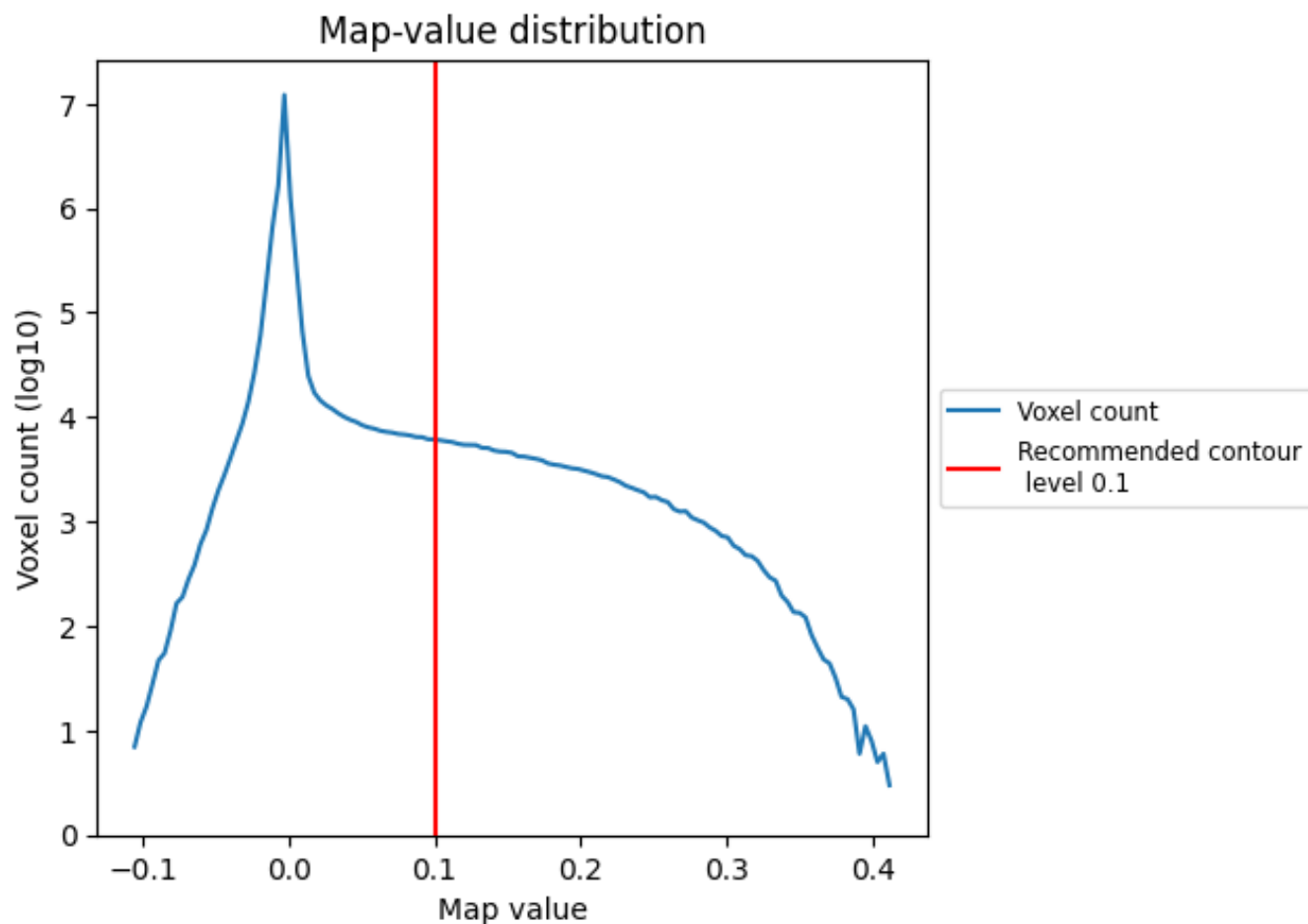
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

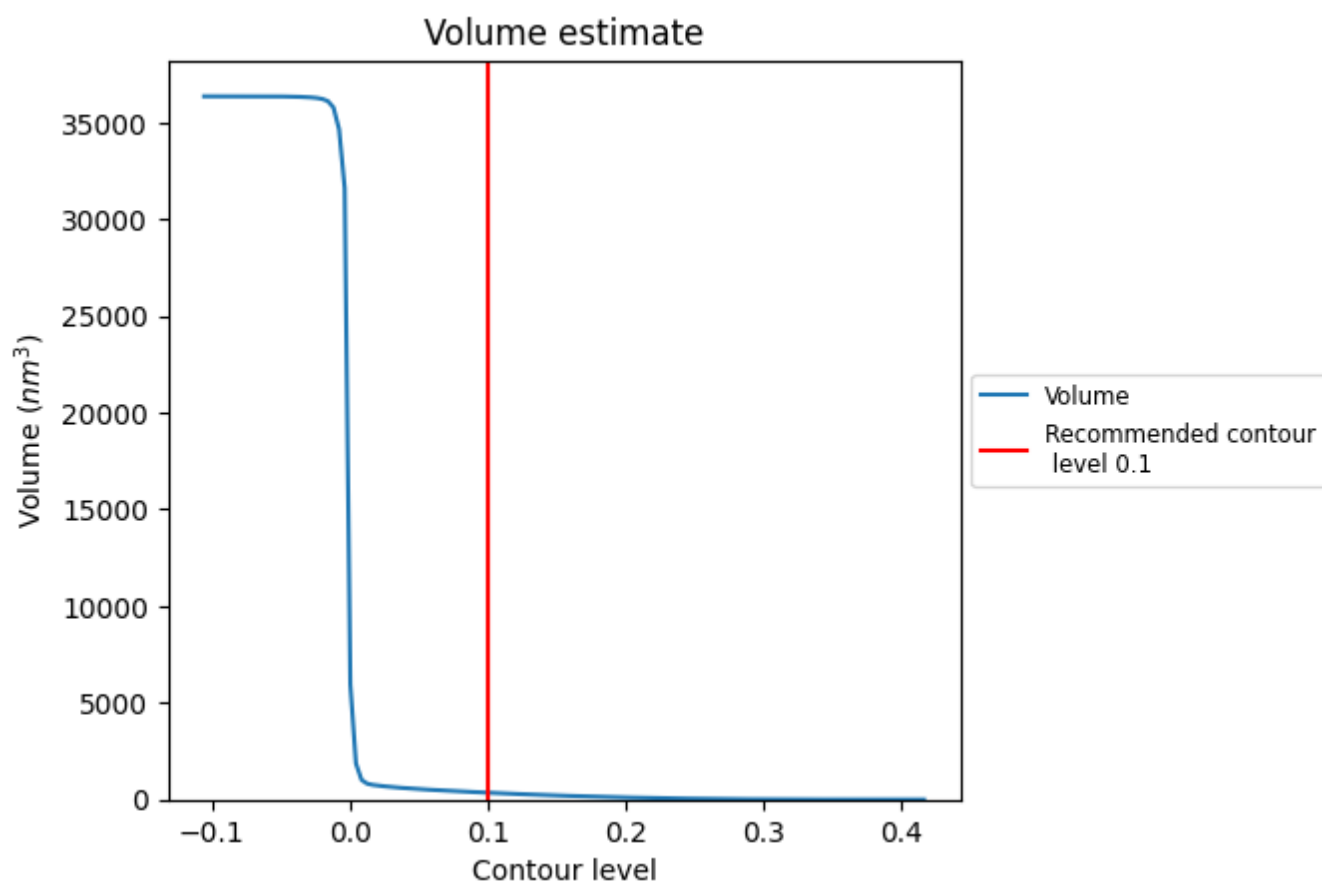
### 7.1 Map-value distribution [i](#)



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](#)

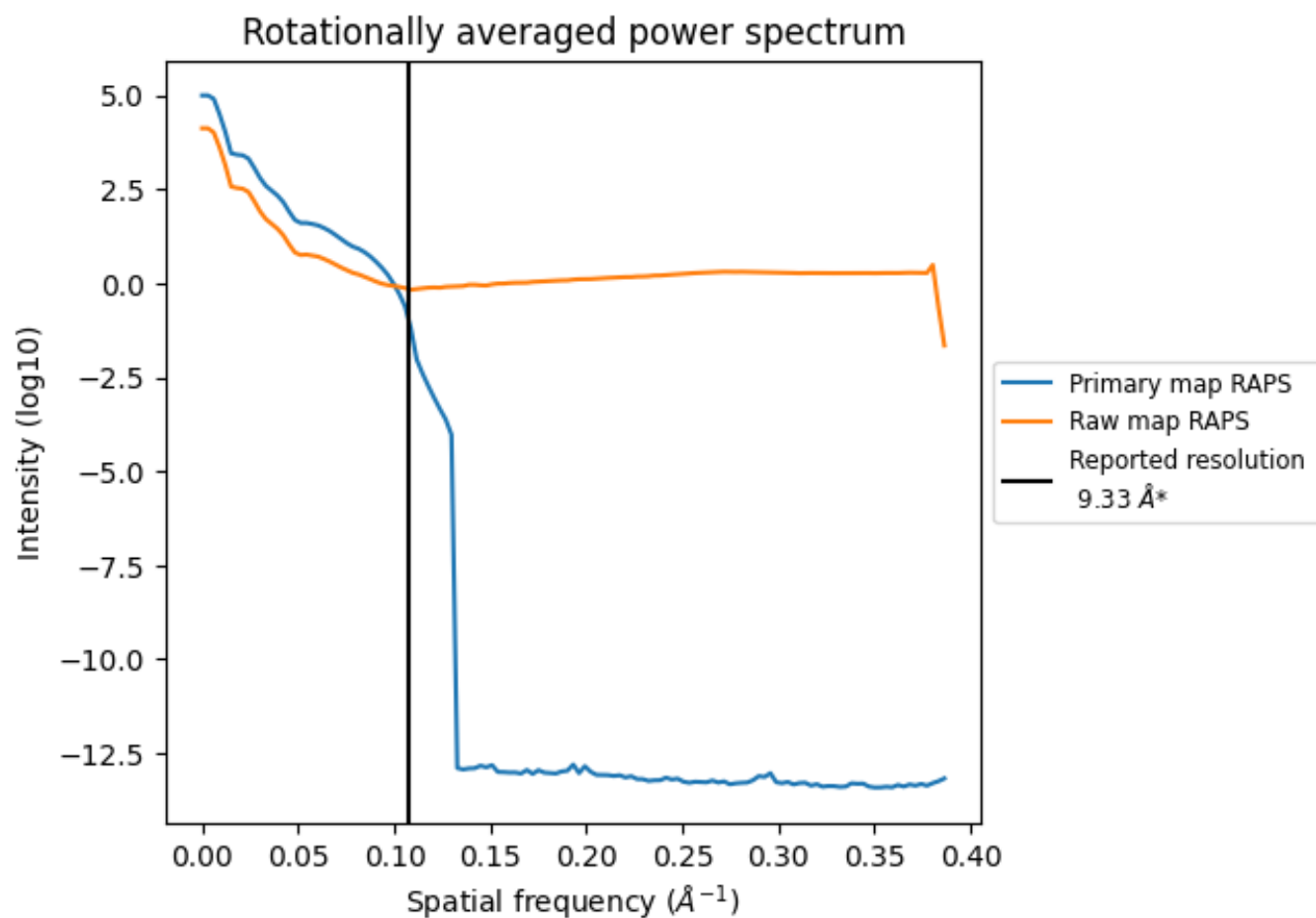


The volume at the recommended contour level is 354  $\text{nm}^3$ ; this corresponds to an approximate mass of 319 kDa.

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 ⓘ



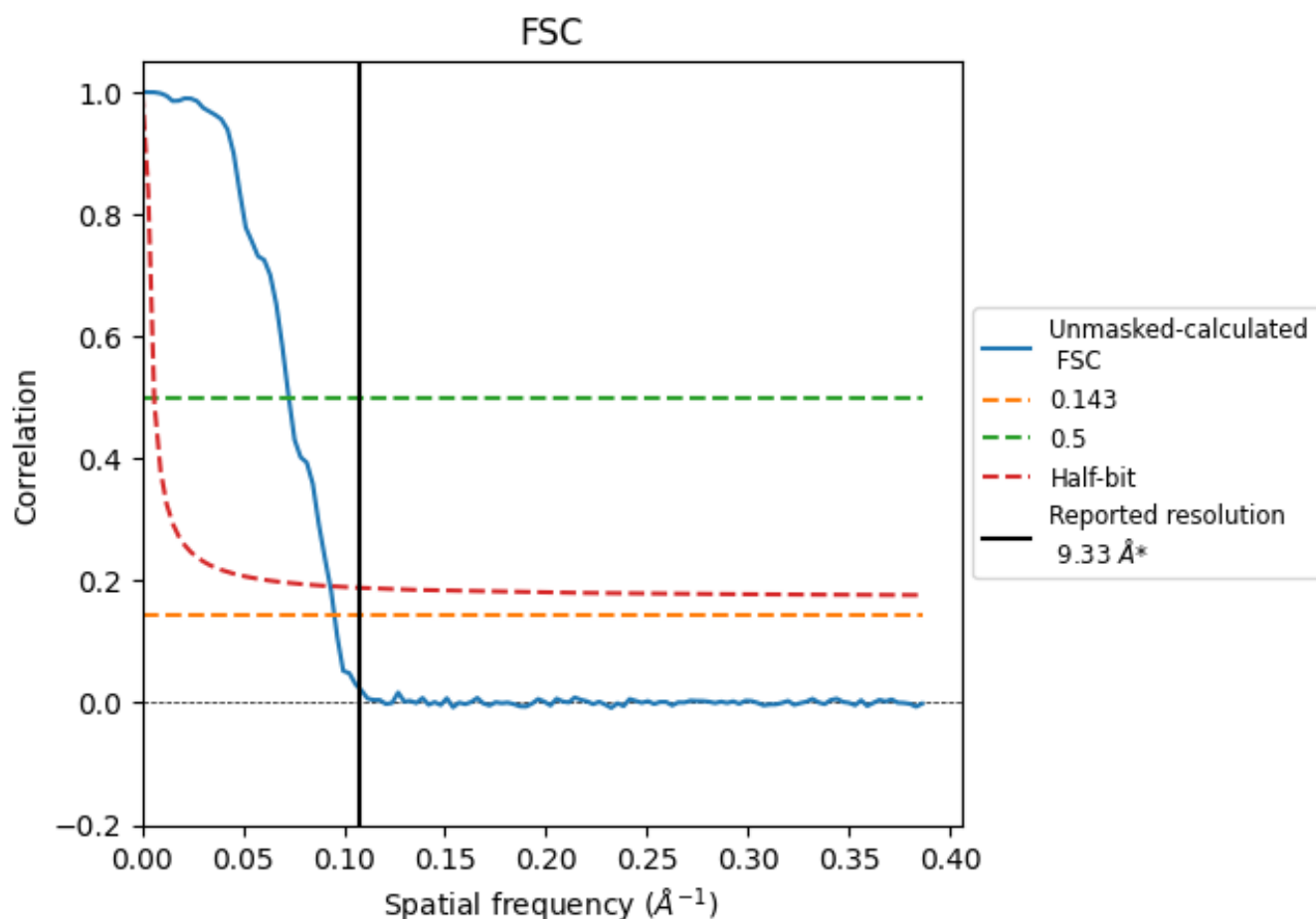
\*Reported resolution corresponds to spatial frequency of 0.107 Å<sup>-1</sup>



## 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 0.107  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.50	13.77	10.74

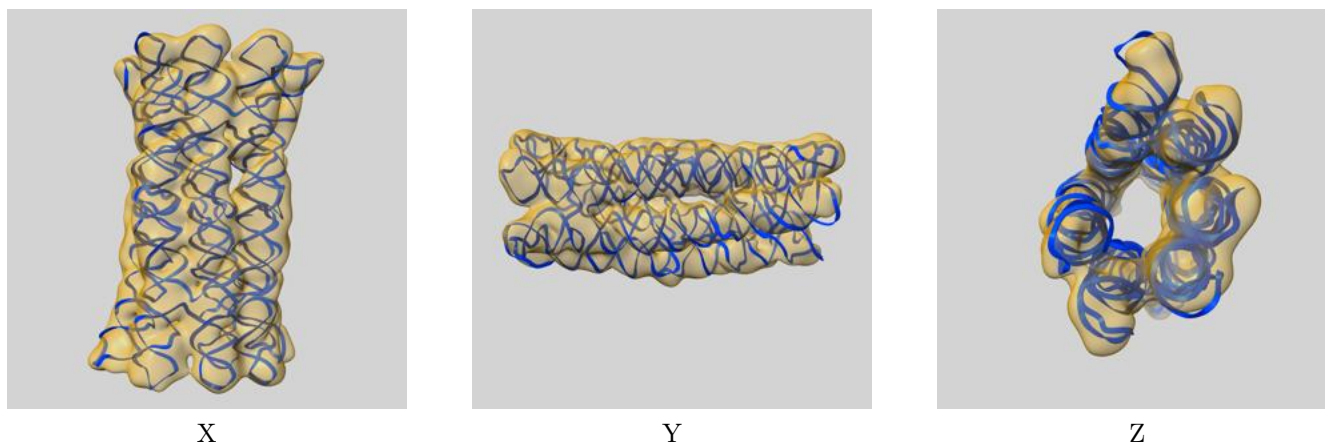
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.50 differs from the reported value 9.33 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53803 and PDB model 9R82. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

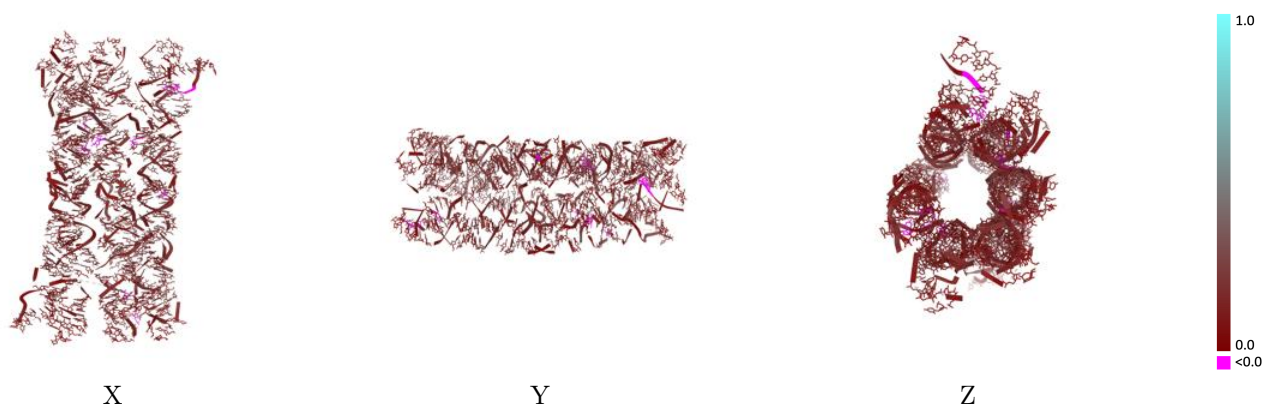
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

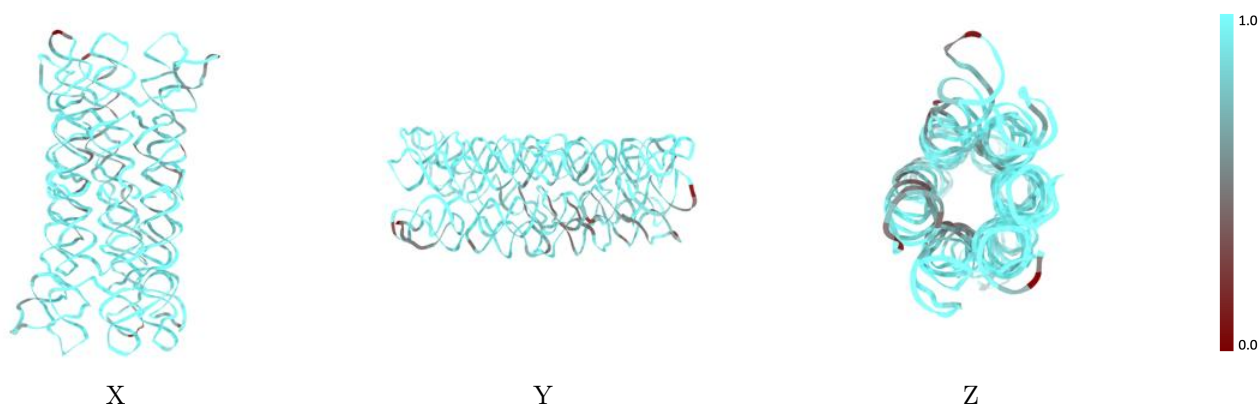


## 9.2 Q-score mapped to coordinate model [i](#)



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.

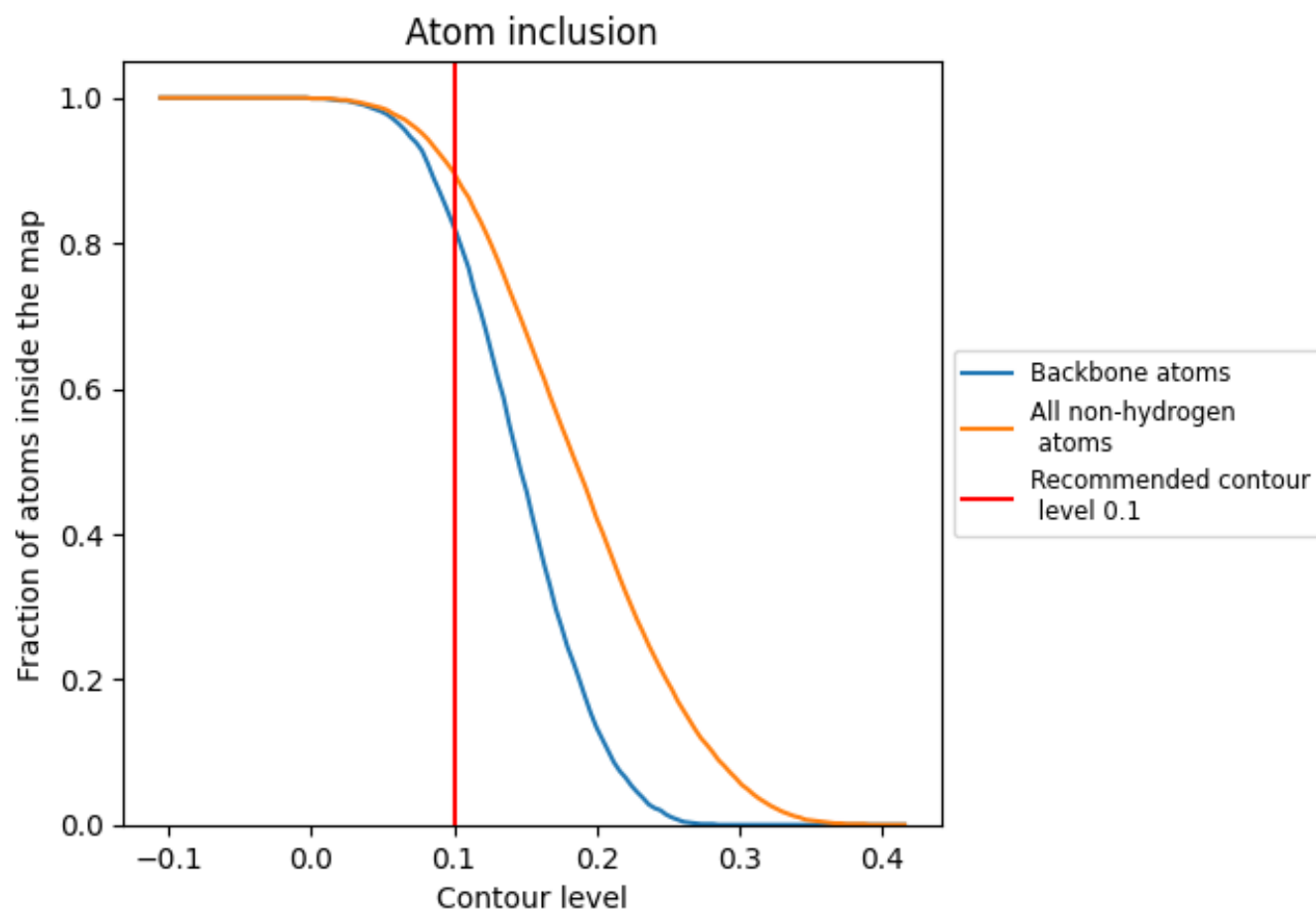
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.1).



## 9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 90% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8970	<div><div></div></div> 0.1410
A	<div><div></div></div> 0.8970	<div><div></div></div> 0.1410

