1 MD and clustering results

This document contains detailed results from the performed MD simulations of DNA triplets. The calculated set of parameters and the measurements on real structures were used to establish groups of structurally isomorphic triplets. Figure 1 serves as a visual explanation of the parameters and their labels used in this document.
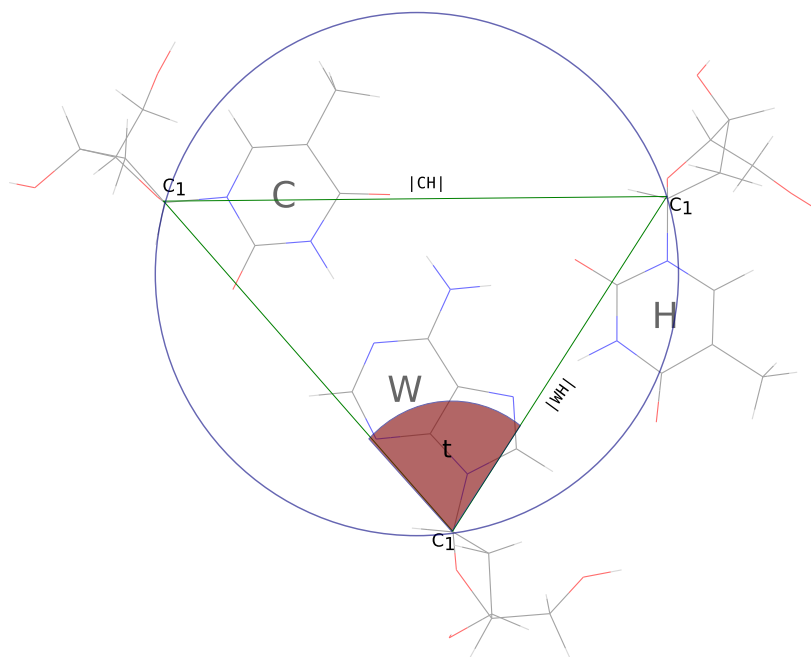

Figure 1: Ilustration of parameters on the $T \cdot A : T$ triplet

1.1 Calculated triplet parameters and groups

	Antiparallel			Parallel	
	t [°]	r [Å]		t [°]	r [Å]
A.A:T	76.5364	7.409632	C.G:C	108.8662	8.897408
A.G:C	125.6857	11.9128	G.G:C	74.82808	7.161497
C.A:T	72.08654	5.563016	G.T:A	125.5032	12.28118
G.G:C	94.1352	7.961633	T.A:T	103.7168	7.896785
T.A:T	72.20278	6.379035	T.C:G	70.47479	6.469698
T.C:G	93.85905	7.441224	T.G:C	77.89392	6.630192

DTN.DAN:DTN-0

DCN.DAN:DTN-0

DAN.DAN:DTN-0

DTN.DCN:DGN-0

DGN.DGN:DCN-0

DAN.DGN:DCN-0

4   3   2   1   0
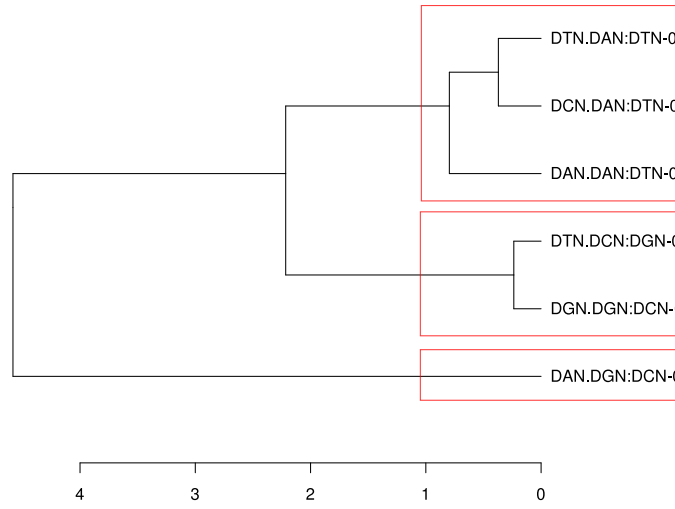
Figure 2: Groups for antiparallel triplets

DTN.DAN:DTN-1

DCN.DGN:DCN-1

DGN.DTN:DAN-1

DTN.DGN:DCN-1

DGN.DGN:DCN-1

DTN.DCN:DGN-1

5   4   3   2   1   0
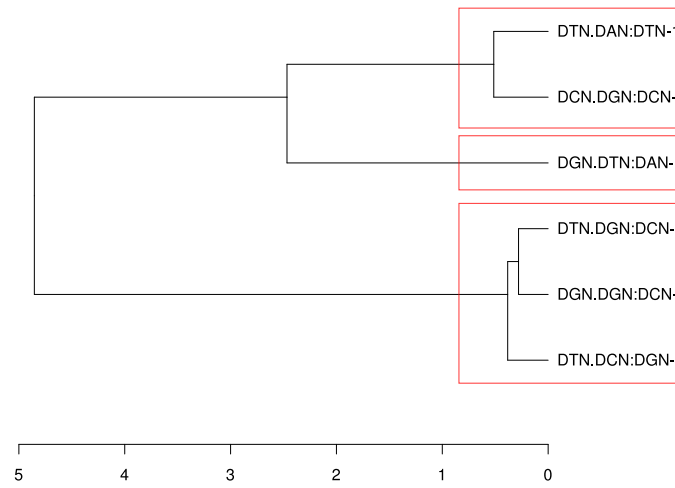
Figure 3: Groups for parallel triplets

2   Measurements

Structure 135D		
$\lvert CH \rvert$ [Å]	$\lvert WH \rvert$ [Å]	t [°]
11.357	9.986	70.4
14.282	11.064	81.8
14.168	11.241	82.8
12.011	9.528	75.0
14.094	11.132	80.7
14.014	11.598	78.5
11.902	9.629	72.7

Structure 149D		
$\lvert CH \rvert$ [Å]	$\lvert WH \rvert$ [Å]	t [°]
14.421	8.527	97.8
14.705	8.503	100.2
14.919	8.947	100.4
14.479	9.631	92.4
14.908	8.713	102.6
14.951	8.660	101.1
14.267	8.548	94.3

Structure 1BCB		
$\lvert CH \rvert$ [Å]	$\lvert WH \rvert$ [Å]	t [°]
14.402	8.547	96.7
14.816	8.645	98.2
14.518	8.343	99.3
14.968	8.169	102.0
14.474	8.222	99.8
14.810	8.442	100.0

Structure 1D3X		
$\lvert CH \rvert$ [Å]	$\lvert WH \rvert$ [Å]	t [°]
15.169	9.124	99.0
14.813	8.607	97.6
14.164	8.850	89.5
13.793	8.902	88.6
14.691	8.949	98.6
14.909	8.922	97.6
14.406	8.929	93.7
15.092	8.667	102.9