

WebTetrado

your assistant in the G4 space

BY MICHAŁ ŻURKOWSKI

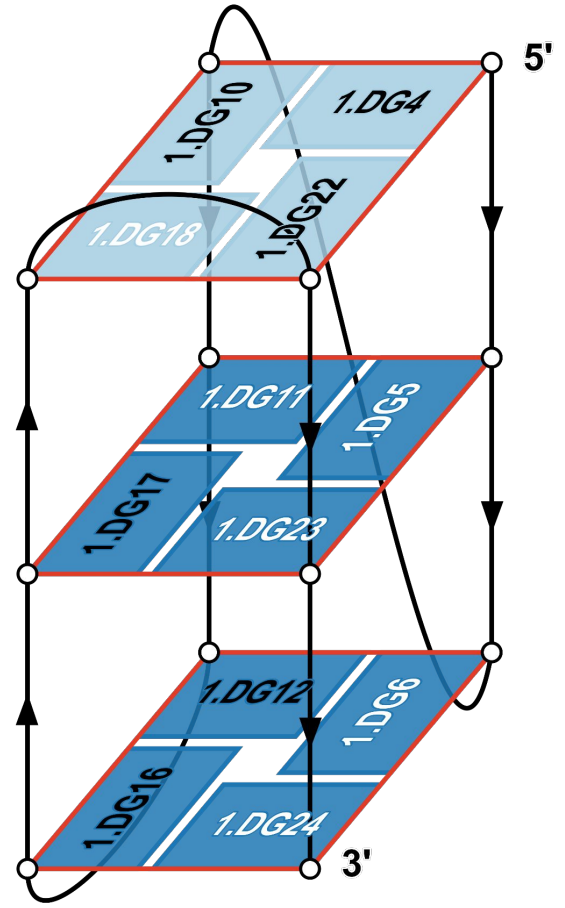
JOINT WORK WITH BARTOSZ ADAMCZYK, TOMASZ ŻOK, MARTA SZACHNIUK

RNA/DNA structure

- Motifs
 - Base pairs
 - Sequence and Chain
 - Nucleotides - C U/T A G
 - Atoms

- Tetrads:

No.	Sequence	Sequence (full names)	ONZ class	Tetrad combination	Planarity [Å]
1	GGGG	1.DG4-1.DG22-1.DG18-1.DG10	O-	Vb	0.17
2	GGGG	1.DG5-1.DG23-1.DG17-1.DG11	O+	Va	0.10
3	GGGG	1.DG6-1.DG24-1.DG16-1.DG12	O+	Vla	0.18



2HY9 - 2.5D structure layer diagram (by DrawTetrado)

RNA/DNA structure

- Base pairs
 - Sequence and Chain
 - Nucleotides - C U/T A G
 - Atoms

- Dot-Bracket:

AAAGGGTTAGGGTTAGGGTTAGGGAA

...([{...(((...))...})]})..

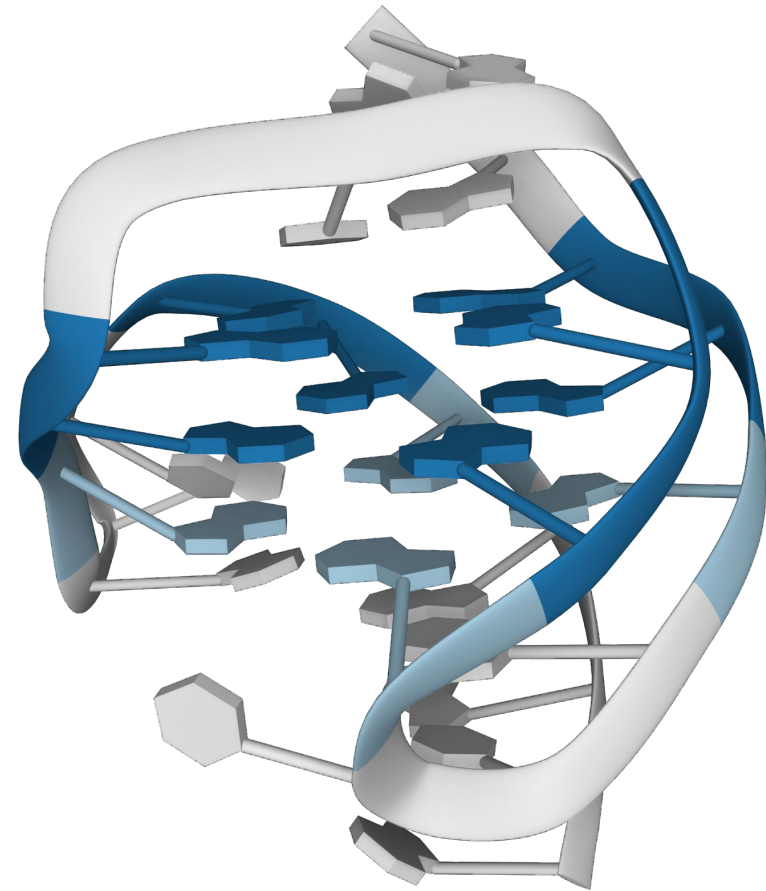
...([{...})]})...(((...)))..



2HY9 - 2D Structure arc diagram (by R-chie)

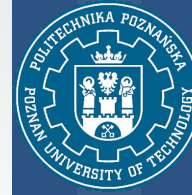
RNA/DNA structure

- Structure
 - Motifs
 - Base pairs
 - Sequence and Chain
 - Nucleotides - C U/T A G
 - Atoms
- Directly connected to biological function of the molecule.



2HY9 - 3D structure cartoon model (by Mol*)

Data Aggregators



Protein Data Bank

The screenshot shows the PDB website with a navigation bar at the top containing links for Deposit, Search, Visualize, Analyze, Download, Learn, More, Documentation, and Careers. A search bar is present with the text "Enter search term(s), Entry ID(s), or sequence". Below the search bar, there are statistics: "200,708 Structures from the PDB" and "1,000,357 Computed Structure Models (CSM)". A sidebar on the left lists navigation options: Welcome, Deposit, Search, Visualize, Analyze, Download, and Learn. The main content area features a "January Molecule of the Month" section with a blue molecular model and the caption "Plastic-eating Enzymes". Below this, there is a "COVID-19 CORONAVIRUS Resources" section with a graphic showing "200000 Structures in the Protein Data Bank".

ONQUADRO

The screenshot shows the ONQUADRO website with a navigation bar at the top containing links for Home, Statistics, Help, About, and Cite us. The main content area features a heading "ONQUADRO" and a paragraph describing the database: "ONQUADRO database collects tetrads, quadruplexes, and G4-helices found in PDB-deposited structures of nucleic acids. It stores their sequences, secondary and tertiary structures, and motif-specific description including planarity, rise and twist parameters, ONZ classification, Webba da Silva geometric formalism, dot-bracket encoding, arc diagrams, etc. Graphical 2D and 3D views complement their characteristics." Below this, there is a section with the text "Click on one of the options below to see the list of entries." and four buttons labeled "Tetrads", "Quadruplexes", "G4Helices", and "Structures", each accompanied by a corresponding 3D molecular model.

WebTetrado webtetrado.cs.put.poznan.pl

Upload DNA/RNA 3D structure

From example collection:

2HY9

6RS3

1JJP

6FC9

1MDG

RNA G-Quadruplex in solution

From local drive:



Click or drag file to this area to upload

*.cif, *.pdb

or

From Protein Data Bank:

PDB ID eg. 1D59

Additional settings

Analyze the model with the number:

Restrict the search to G-tetrads: Yes

Detect tetrads with cWH pairings only: No

Accept stacking mismatch for how many nts:

Reorder chains to optimize ONZ: Yes

- PDB ID
- .cif or .pdb file

- Input parameters

WebTetrado

- Save link or task ID for later
- Results kept for 1 week.

Show the results of completed task

Task id: *0143b990-a02d-11ed-b321-0242ac1e0003*



WebTetrado - Analysis

- EITetrado
 - Base Pairs - Using RNApolis
 - Tetrads and ONZ classes
 - Tracts
 - Loops
 - Quadruplexes



Github: [tzok/eltetrado](https://github.com/tzok/eltetrado)

Basic data

Structure visualizations

Tetrads

Loops

Chi angles

Tetrad pairs

Base pairs

Nucleotides

WebTetrado

A(GGGG) PENTAD-CONTAINING DIMERIC DNA QUADRUPLEX INVOLVING STACKED G(ANTI)G(ANTI)G(ANTI)G(SYN) TETRADS

N4-Helix 1

Quadruplex 1

Basic data

PDB ID:	1JJP	Molecule:	DNA	Experimental method:	SOLUTION NMR
Type (by no. of strands):	bimolecular	No. of tetrads:	4	ONZM class:	Mh*
Tetrad combination:	VIII [⊙]				

Basic data

Structure visualizations

Tetrads

Loops

Chi angles

Tetrad pairs

Base pairs

Nucleotides

2D structure (dot-bracket):

```
GGGAGGTTTGGGAT - GGGAGGTTTGGGAT
(( ( . )) . . . (( ( . )) . . . - [[ [ { . ] ( . . . ] ] } . .
([ [ { . [ ( . . . ] ] } . . - ] ( [ . ] . . . [ ] ] . .
```

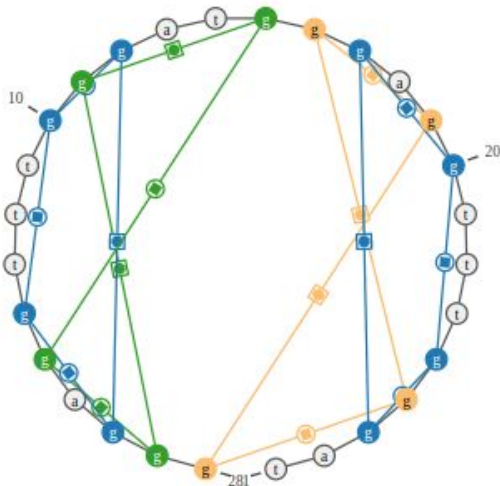
Color codes



Classic diagram (by VARNA)

Show canonical base pairs outside tetrads: No

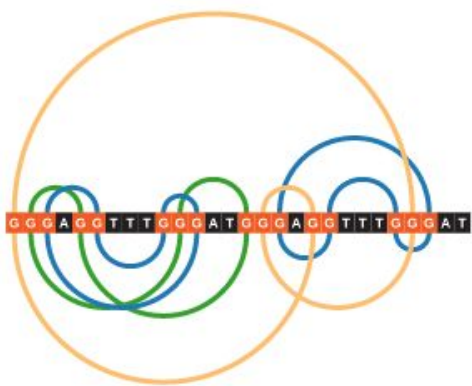
Show non-canonical base pairs outside tetrads: No



Download

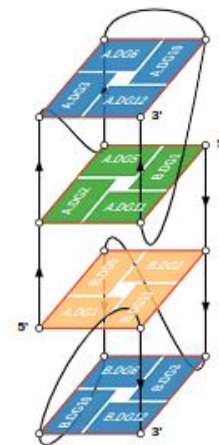
Arc diagram (by R-chie)

Show canonical base pairs outside tetrads: No



Download

Layer diagram (by DrawTetrado)



Download

Basic data

Structure visualizations

Tetrads

Loops

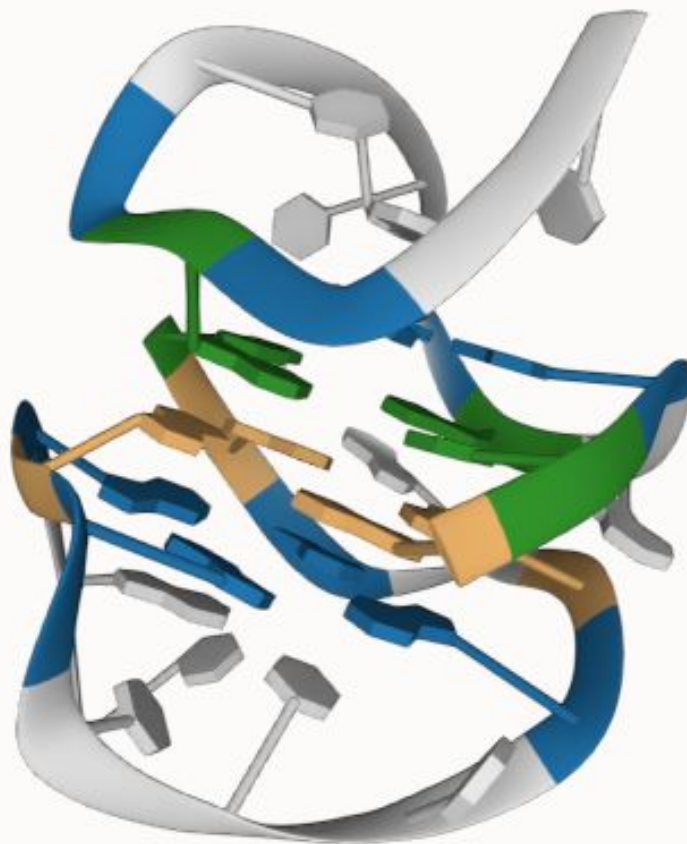
Chi angles

Tetrad pairs

Base pairs

Nucleotides

3D structure (by Mol*)



Basic data

Structure visualizations

Tetrads

Loops

Chi angles

Tetrad pairs

Base pairs

Nucleotides

Tetrads

Number	Sequence	Sequence (full names)	ONZ class	Tetrad combination	Planarity [Å]	Download
1	GGGG	A.DG3-A.DG6-A.DG10-A.DG12	O+	VIIIa [Ⓞ]	0.11	
2	GGGG	A.DG2-A.DG5-B.DG1-A.DG11	N+	VIIIa [Ⓞ]	0.22	
3	GGGG	A.DG1-B.DG5-B.DG2-B.DG11	Z-	VIIIa [Ⓞ]	0.22	
4	GGGG	B.DG10-B.DG6-B.DG3-B.DG12	O+	VIIIa [Ⓞ]	0.11	

< 1 >

 Download CSV

Loops

Number	Sequence	Sequence (full names)	Loop length	Loop type
1	A	A.DA4	1	propeller-
2	TTT	A.DT7, A.DT8, A.DT9	3	lateral-
3	A	B.DA4	1	propeller-
4	TTT	B.DT7, B.DT8, B.DT9	3	lateral-

Download CSV



Basic data

Structure visualizations

Tetrads

Loops

Chi angles

Tetrad pairs

Base pairs

Nucleotides

Chi angles

Tetrad number	Nucleotide 1	Nucleotide 2	Nucleotide 3	Nucleotide 4
1	A.DG3: -126.26° / anti	A.DG6: -115.59° / anti	A.DG10: 94.11° / anti	A.DG12: -125.99° / anti
2	A.DG2: -152.93° / anti	A.DG5: -158.60° / anti	B.DG1: 97.81° / anti	A.DG11: 169.70° / anti
3	A.DG1: 97.76° / anti	B.DG5: -158.57° / anti	B.DG2: -152.81° / anti	B.DG11: 169.74° / anti
4	B.DG10: 94.18° / anti	B.DG6: -115.65° / anti	B.DG3: -126.35° / anti	B.DG12: -125.92° / anti



Download CSV



Basic data

Structure visualizations

Tetrads

Loops

Chi angles

Tetrad pairs

Base pairs

Nucleotides

Tetrad pairs

Number	Tetrad sequences	Twist [°]	Rise [Å]	Strands
1	A.DG3-A.DG6-A.DG10-A.DG12 A.DG2-A.DG5-B.DG1-A.DG11	35.49	3.09	hybrid
2	A.DG2-A.DG5-B.DG1-A.DG11 A.DG1-B.DG5-B.DG2-B.DG11	22.30	3.06	hybrid
3	A.DG1-B.DG5-B.DG2-B.DG11 B.DG10-B.DG6-B.DG3-B.DG12	34.84	3.09	parallel



Download CSV



Basic data

Structure visualizations

Tetrads

Loops

Chi angles

Tetrad pairs

Base pairs

Nucleotides

Base pairs

Number ↕	Stericity	3'-edge	5'-edge	Nucleotide 1	Nucleotide 2	In tetrad ↕
1	cis	Watson-Crick-Franklin	Hoogsteen	A.DG1	B.DG5	✓
2	cis	Hoogsteen	Watson-Crick-Franklin	A.DG1	B.DG11	✓
3	trans	Hoogsteen	Sugar	A.DG2	A.DA4	
4	cis	Hoogsteen	Watson-Crick-Franklin	A.DG2	A.DG5	✓
5	cis	Watson-Crick-Franklin	Hoogsteen	A.DG2	A.DG11	✓
6	cis	Hoogsteen	Watson-Crick-Franklin	A.DG3	A.DG6	✓
7	cis	Watson-Crick-Franklin	Hoogsteen	A.DG3	A.DG12	✓
8	cis	Hoogsteen	Watson-Crick-Franklin	A.DG5	B.DG1	✓
9	cis	Hoogsteen	Watson-Crick-Franklin	A.DG6	A.DG10	✓
10	trans	Watson-Crick-Franklin	Watson-Crick-Franklin	A.DT8	A.DA13	



- Basic data
- Structure visualizations
- Tetrads
- Loops
- Chi angles
- Tetrad pairs
- Base pairs
- Nucleotides**

Nucleotides

Number	Symbol	Full name	Chi angle (value) [°]	Chi angle (type)
1	G	A.DG1	97.76	anti
2	G	A.DG2	-152.93	anti
3	G	A.DG3	-126.26	anti
4	A	A.DA4	-91.36	anti
5	G	A.DG5	-158.60	anti
6	G	A.DG6	-115.59	anti
7	T	A.DT7	-112.93	anti
8	T	A.DT8	-177.69	anti
9	T	A.DT9	-117.39	anti
10	G	A.DG10	94.11	anti

Future work

Thanks for listening!



WebTetrado: <https://webtetrado.cs.put.poznan.pl>

Publication pending

B. Adamczyk, M. Zurkowski, M. Szachniuk, T.Zok.

“WebTetrado: a webserver to explore quadruplexes in nucleic acid 3D structures”

EITetrado: <https://github.com/tzok/eltetrado>

T. Zok et al. (2020) “EITetrado: A Tool for Identification and Classification of Tetrads and Quadruplexes.”
BMC Bioinformatics. doi:10.1186/s12859-020-3385-1

DrawTetrado: <https://github.com/michal-zurkowski/drawtetrado>

Zurkowski et al. (2022) “DrawTetrado to create layer diagrams of G4 structures”. Bioinformatics
doi.org/10.1093/bioinformatics/btac394

ONQUADRO: <https://onquadro.cs.put.poznan.pl>

T. Zok et al. (2022) “ONQUADRO: a database of experimentally determined quadruplex structures”,
Nucleic Acids Research; doi:10.1093/nar/gkab1118