

Annotation and Validation of Nucleic Acid Structures (and Models)

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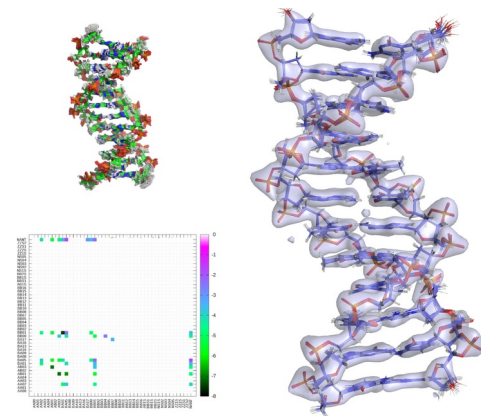
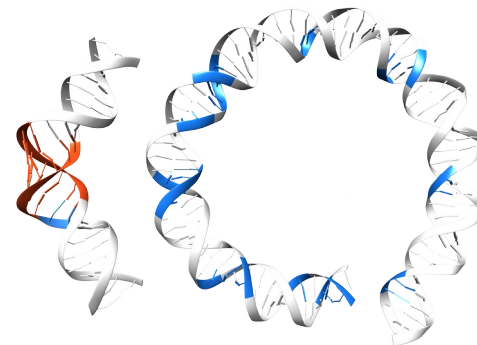
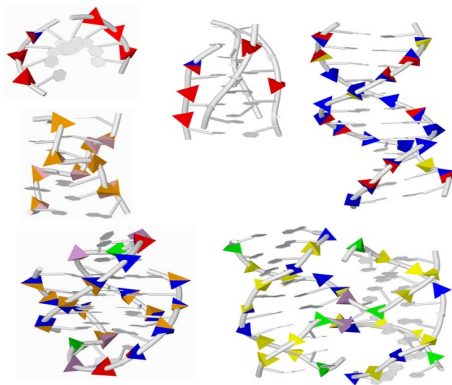
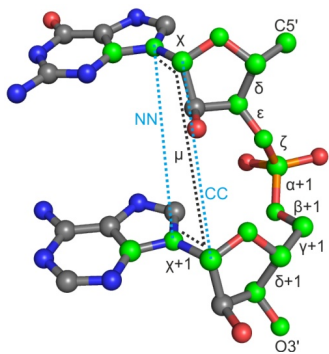


3DBioInfo community

Nucleic Acids

Structural alphabets (NtC and CANA) for conformational analysis of nucleic acids (DNA and RNA).

- Annotation
- Validation
- Model building
- Modeling
- Enhanced sampling MD
- Refinement



DNATCOTM v4.1
Assignment of DNA and RNA conformers

Submit own PDB or CIF file

Coordinates Soubor newybrán

Electron density map (optional) Soubor newybrán

Enter PDB ID (e.g. 1bna)

<https://dnatco.datmos.org>

job **Control** Examples

State: Job has finished
Step: 20
Total steps: 20
User interface mode: **Simple**

Name: **Tetraloop**

Compound definition

Chain	First residue no.	Type	Sequence
A	1	RNA	UACUAGAUA

Double helices

Chain	First residue	Last residue	Chain	First residue	Last residue
A	2639	2642	A	2644	2648

Base Interactions

Chain	Residue	Edge	Chain	Residue	Edge	Orientation
A	2639	Watson-Crick	A	2639	Watson-Crick	Cis

NICs

Chain	Residue	NIC
A	2639	AA00
A	2642	AA00
A	2643	OP03
A	2643	AA08
A	2644	AA00

Global parameters
Interaction scale factor: 1.00

Ball-and-stick | Cartoon | Download

Show stage | Refresh rate (sec): 10 | Auto:

MMB Output

<https://webmmb.datmos.org>



Protein linkers database

Lead sequence: Tail sequence:

Specify pt: ---LINKER--- Specify pt:

Linker residue count: At most: Minimum: Linker span (Å): Maximum:

Source organism: Expression organism:

Filter: Clear Filter: Clear

Group: Bacteria (20500 links)

Filter: colli

Search

Link to results | Filtering

Linker ID	Linker sequence	L.S. pt	L.S. Span	FoldIndex	Description
1. Q8T8K2_232_237	EEDKE	3.67	11.08	-1.529	N-lysine methyltransferase SETD6
2. Q29BFX_B3_93	DMEDDEEEDG	2.99	14.38	-1.421	Condensin complex subunit 3
3. Q29S6L_176_177	IKKKDQEK	11.28	11.33	-1.362	SH3-containing GBD-like protein 2
4. Q9H4U5_552_558	EQDEEA	3.26	14.22	-1.322	REGULATOR OF NONSENSE TRANSCRIPTS 2

<https://linkers.datmos.org>

libr BROWSE ABOUT PREDICTIONS CONTACTS HOW TO CITE DOWNLOADS WATLAS

WatAA: Atlas of Protein Hydration

Browse

Hydration of the 20 standard amino acids in proteins

Amino-acid (AA) and hydration site (HS) selection

AA	Secondary structure	χ1 rotamer	HS #
Arg	HT	g	HS1

Display/Hide

Atomic positions of the AA with all HS

Water distribution map @ 1σ % occupancy

Water position after QM optimization

Spinning on/off

Viewer width

Statistics

22 AA residues and 53 water molecules (within 3.2 Å) found for Arg_H_g

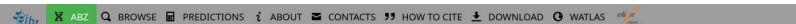
Data for individual HS

HS#	Water position based on data mining				Water position after QM optimization			
	Occupancy	Nearest atom	Distance [Å]	Eint [kcal/mol]	Nearest atom	Distance [Å]	Eint [kcal/mol]	Displacement [Å]
1	0.39	O	2.81	-4.37	O	2.78	-4.44	0.06
2	0.38	NH2	2.74	-3.47	NH2	2.87	-3.86	0.13
3	0.35	NH1	2.64	-4.6	NH1	2.81	-5.65	0.18
4	0.27	NE	2.94	-4.97	NE	2.88	-6.93	1.02
5	0.25	NH1	2.8	-5.07	NH1	2.80	-5.07	0.01

Arg_H_g-HS1

Labels and Measurements

<https://wataa.datmos.org>



WatNA: Online Atlas of DNA Hydration

libr ABZ BROWSE PREDICTIONS CONTACTS HOW TO CITE DOWNLOAD WATLAS

Table 1: Number of water molecules for selected NIC conformers of B-DNA, A-DNA and mixed A/B form.

Nic/seq.	BB00	BB07	AA00	AB01	BA05
A.A	8838	954*	321	177	1053
A.C	4496	107	1100	357	2717
A.G	7208	889*	1111	415	1319
A.T	6148	46	618	588	3542
C.A	5529	2413	939*	1486	774
C.C	5235	529	3326	813*	7
C.G	8275	2834	2103	3775	3
C.T	5126	253	1182	1391	794
G.A	8909	2010	464	315	726
G.C	7612	1884	2725	890*	3456
G.G	10897	3474	2549	422	1243
G.T	7766	166	1758	483	1564
T.A	7082	1958	729	1175	867
T.C	6567	752	993*	672	1933
T.G	8111	2293	693	994*	234
T.T	7866	52	463	842*	1025

Table 2: Number of water molecules for selected NIC

Controls

BB00_C_G

Reference dinucleotide

Hydration sites

Base

Backbone

Hydration distribution

Base o Watline 0.14

Backbone o Watline 0.13

Save view as image

Reset colors

Clip radius 1.00

Reset camera

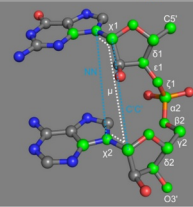
Lighting Default

<https://watna.datmos.org>

HOME HELP TUTORIAL TABLE OF CONFORMERS BROWSE CONFORMERS ABOUT HOW TO CITE DOWNLOAD

DNATCO^[7] v4.1

Assignment of DNA and RNA conformers



Submit own PDB or CIF file

Coordinates Soubor nejvýbrán

Electron density map (optional) Soubor nejvýbrán

Enter PDB ID (e.g. 1bna)

Structure and model of (GGUGCAGUAGGAGACGAACCGCACC) analyzed with <https://dnatco.datmos.org>

Home or other PDB ID

Show reference

Camera radius ratio Map

Selection mode Show difference map

Center view on selection Show all alleles

Show contacts within radius (Å) Transparency


Map as wireframe Signa (diff. map)

Transparency (diff. map)

Click the Summary/Torsions/Similar... tabs for more details.

[Summary](#) [Torsions](#) [Similar](#) [Settings](#) [Browse](#) [Download](#)

Results of the assignment of 26 detected steps in 1 model(s), can be also downloaded as [csv](#) or [json](#) file. Found **24/26** steps in 0-0.5/0.5-1.0/1.0-Å Cartesian rmd from reference. Average confid **72**, percentile **93**.



Click a row in table or a step in viewers for analysis of results. Click column headers to sort data.

Step name	CANA	NC	confid	rmd
1q93_A_G2_G3	AAA	AA00	81	0.13
1q93_A_G3_U4	AAA	AA00	78	0.09
1q93_A_U4_G5	AAA	AA00	89	0.65
1q93_A_G5_C6	AAA	AA00	87	0.22
1q93_A_C6_U7	AAA	AA00	59	0.33
1q93_A_U7_C8	AAA	AA08	64	0.29
1q93_A_C8_A9	ZZZ	ZZ01	78	0.30
1q93_A_A9_G10	OPN	OP23	74	0.21
1q93_A_G10_U11	OPN	OP15	91	0.15
1q93_A_U11_A12	AAA	AA00	70	0.30
1q93_A_A12_G13	AAA	AA08	60	0.51
1q93_A_G13_G14	AAA	AA00	66	0.22
1q93_A_G14_A15	OPN	OP93	96	0.30
1q93_A_A15_G16	AAA	AA00	50	0.37
1q93_A_G16_A17	AAA	AA00	64	0.26
1q93_A_A17_C18	Aww	AA05	80	0.20
1q93_A_C18_G19	AAA	AA08	54	0.44
1q93_A_G19_A20	OPN	OP98	91	0.17
1q93_A_A20_A21	AAA	AA08	78	0.20
1q93_A_A21_G22	AAA	AA03	61	0.25
1q93_A_G22_G23	Aww	AA01	73	0.18
1q93_A_G23_G24	AAA	AA08	53	0.46
1q93_A_G24_G25	AAA	AA00	76	0.18
1q93_A_G25_A26	AAA	AA00	36	0.14
1q93_A_A26_C27	AAA	AA08	81	0.18
1q93_A_C27_G28	AAA	AA00	86	0.17

Steps with non-standard or missing atoms have not been assigned, description of conformers is defined in the [table](#).

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Conformers: A B mB mC mN SSN N