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DNATCO

https://dnatco.datmos.org↗

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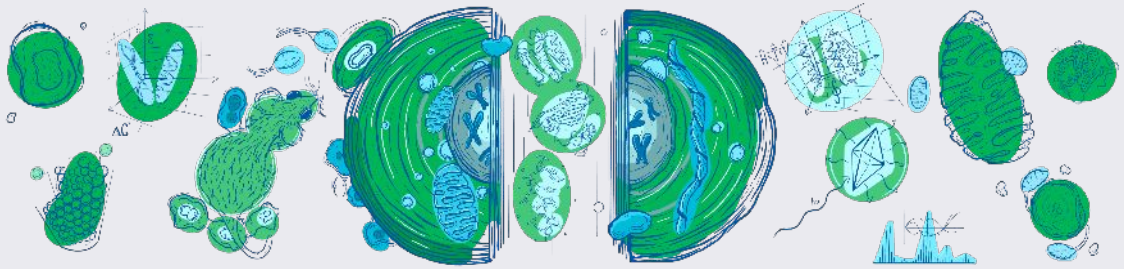
https://github.com/cernylab



Benasque RNA 3D session 2026/07/14

DNATCO: FAQs

Q: Does it mean anything?
A: For sure it used to be a clever acronym, in the meantime forgotten.

- We only know that it is not about “DNA” (anymore).
- AI called to assistance, pick yours:
  - DiNucleotide Analysis and Conformations
  - DiNucleotide Alphabet of Torsional COnformers

Q: How do you pronounce it?
A: It is a bit of a tongue twister, right? You can follow Django here:

- “the D is silent”

Q: What is it good for?

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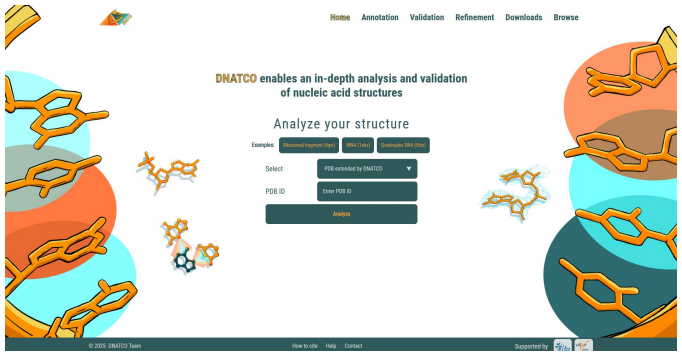
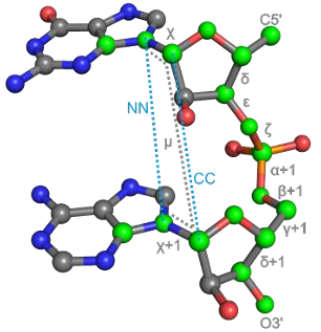
DNA and RNA 3D Structures: From Complexity to Clarity

DNATCO: user-friendly toolbox for annotation, validation, modeling, and refinement of nucleic acid structures

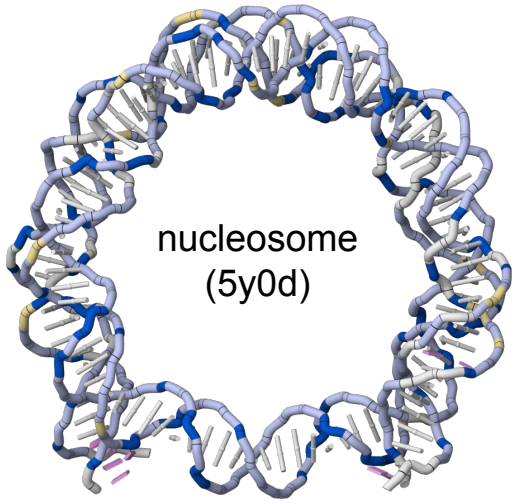


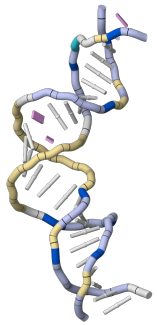
https://dnatco.datmos.org

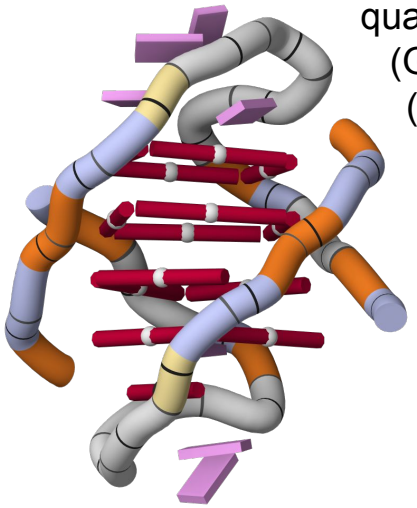


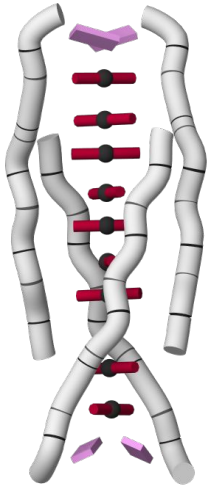
- Černý J, Malý M, Božíková P, Prchalová T, Svoboda J, Biedermannová L, Schneider B. "DNATCO v5.0: integrated web platform for 3D nucleic acid structure analysis." *Nucleic Acids Res.* ***2026***, https://doi.org/10.1093/nar/gkaf1491
- Černý J, Božíková P, Svoboda J, Schneider B. "A unified dinucleotide alphabet describing both RNA and DNA structures." *Nucleic Acids Res.* ***2020***, https://doi.org/10.1093/nar/gkaa383
- Černý J, Nicholls RA, Brzezinski D, Berman HM, Gilski M, Joosten RP, Kowiel M, Lawson CL, Moriarty NW, Richardson JS, Schneider B, Vonrhein C, Williams CJ, Jaskólski M, Egli M. "New targets and procedures for validating the valence geometry of nucleic acid structures." *Nucleic Acids Res.* ***2026***, https://doi.org/10.1093/nar/gkaf1335

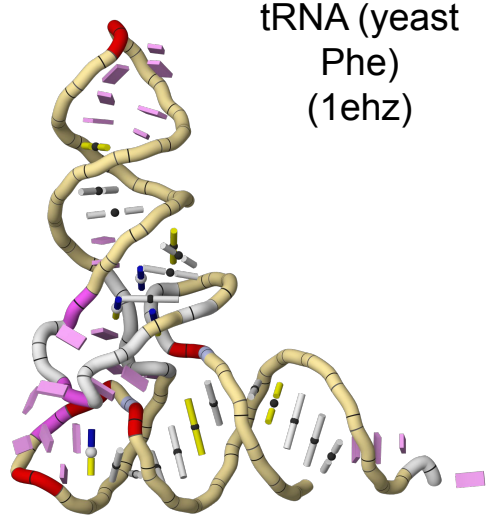
Visual annotation of backbone conformations and base pairing

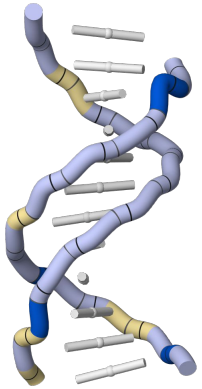

nucleosome
(5y0d)

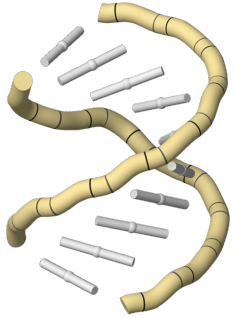

TF-bound DNA
(4roc)

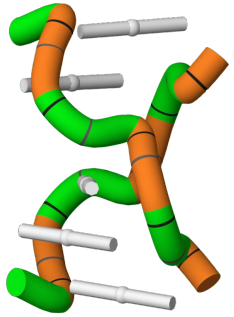

quadruplex
(G-rich)
(5hix)

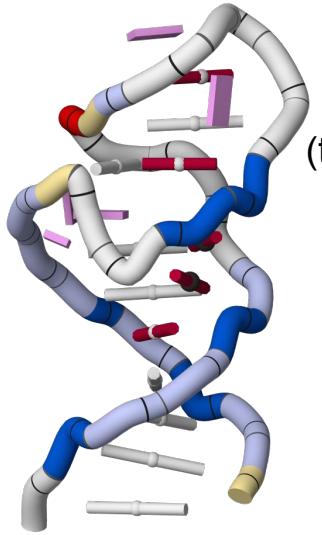

i-motif
(C-rich)
(1i9k)

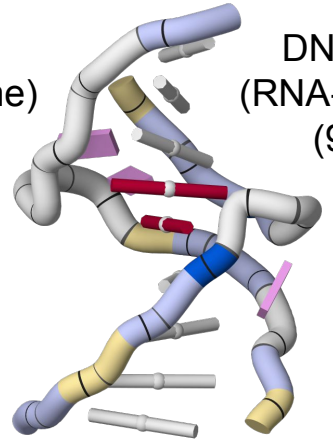

tRNA (yeast
Phe)
(1ehz)

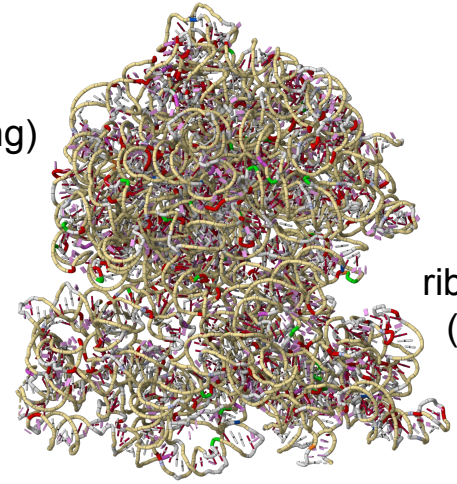

B-form
(1bna)


A-form
(440d)


Z-form
(4hig)


aptamer
(theophylline)
(8k0t)


DNAzyme
(RNA-cleaving)
(9k8o)


ribosome
(8b0x)

(online demo)

https://dnatco.datmos.org

https://dnatco.datmos.org/?cifcode=1ehz&stepName=1ehz_A_G_22_A_23

https://dnatco.datmos.org/?cifcode=1ehz&basePair=1ehz_A_A_9_A_A_23

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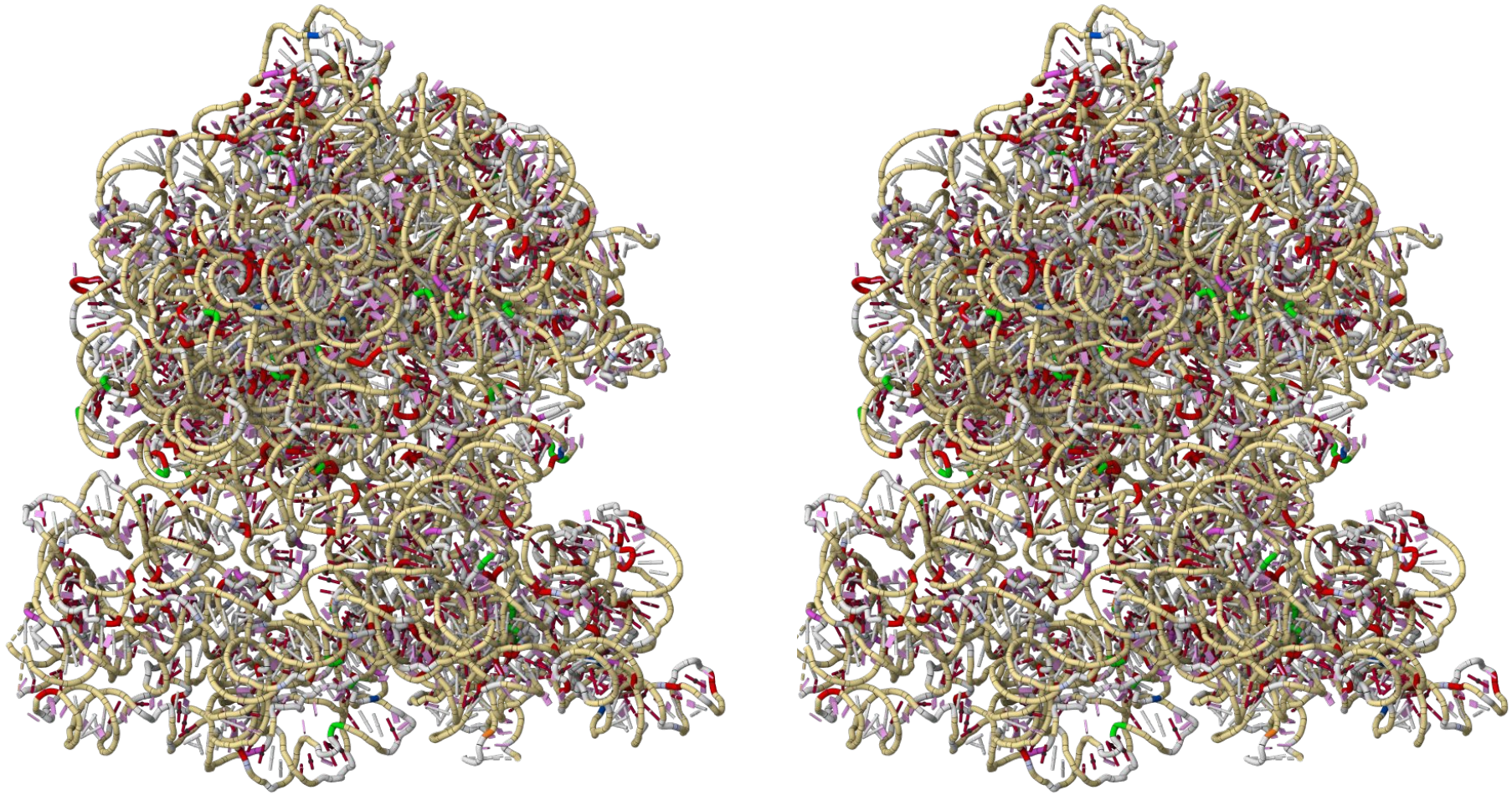
https://dnatco.datmos.org/?cifcode=1ehz&residue=1ehz_A_A_21&angle=C4%27_C3%27_O3%27

(to be continued on slide 11)

Ribosome (8b0x, 1.55Å cryoEM)



A
B
BII
miB
Z
IC
OPN
SYN
N

A
B
BII
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Z
IC
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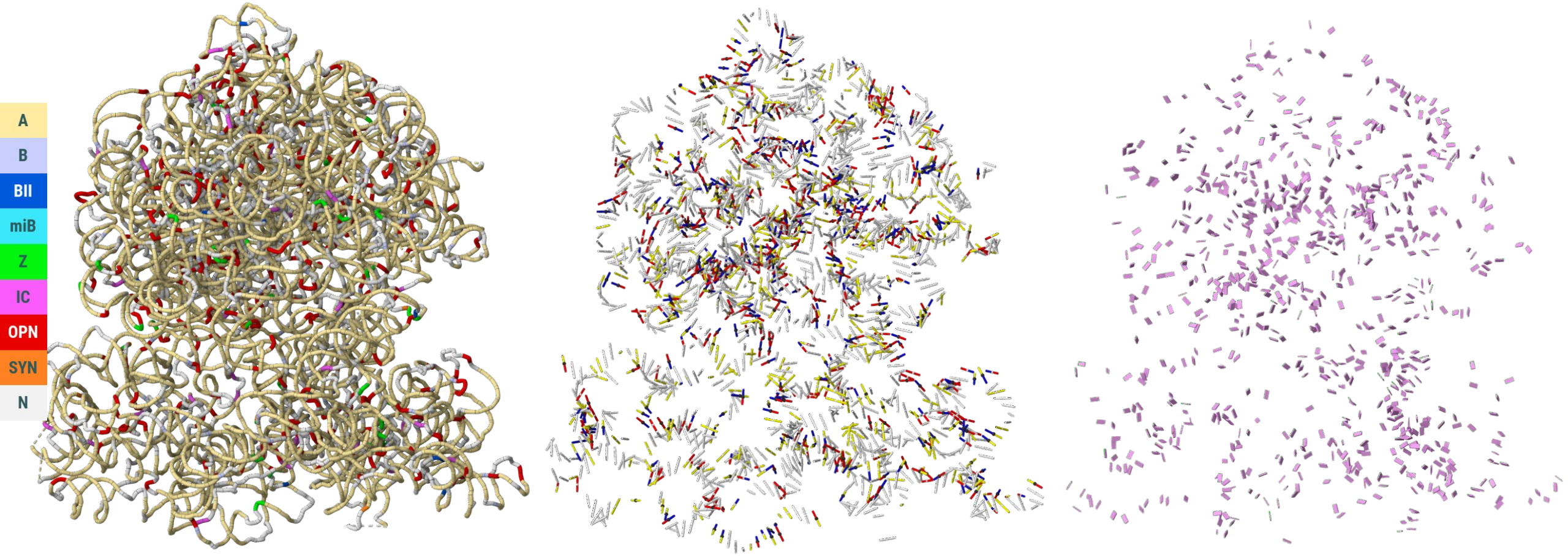
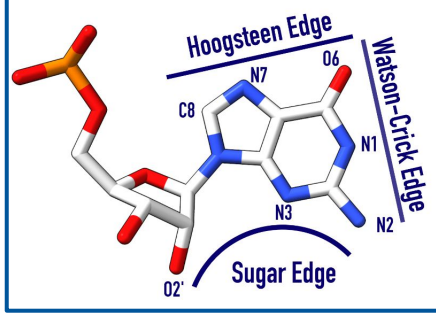
SYN
N

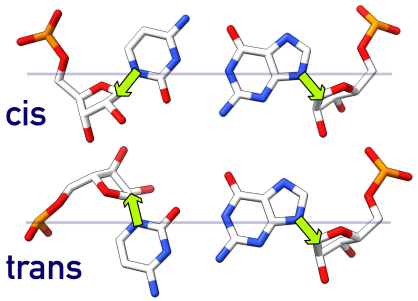
Ribosome (8b0x, 1.55Å cryoEM)

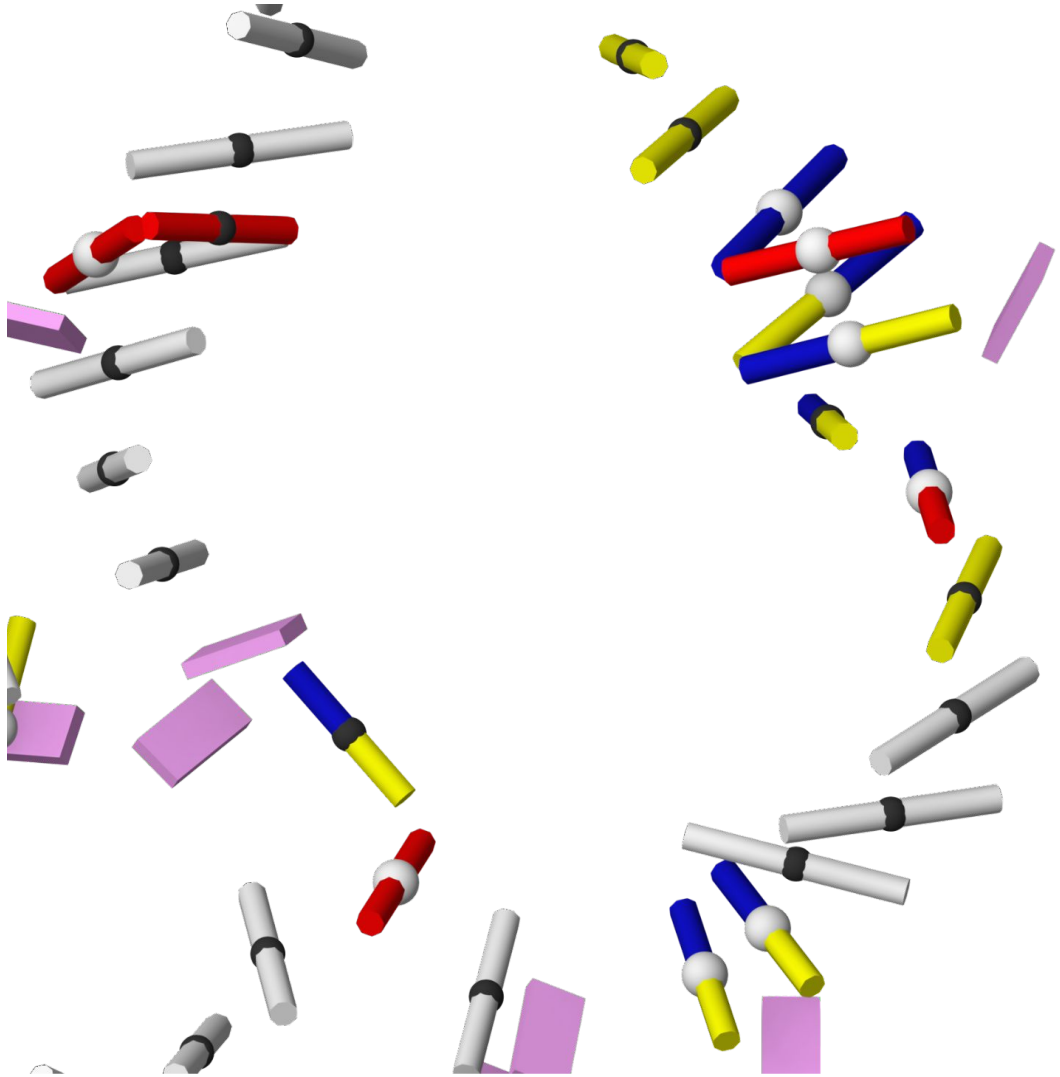


Base pairing motifs (8b0x, 1.55Å cryoEM ribosome)

cWW (G-C, A-U)
W
H
S
cis
trans
unpaired







Validation and refinement of NA conformations

Overall Quality
Conformer Quality
Base Pairs
Step Torsions
Similarity Plot
RSCC/RMSD Plot
Bond Lengths & Angles
Downloads
Help
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1EHZ The crystal structure of yeast phenylalanine tRNA at 1.93 A resolution
Resolution 1.9 Å (Low: 40.0)

Conformer quality

Table of assigned dinucleotide NtC classes

Chain	Step	NtC	CANA	Confal score	RMSD
A	M2G26 C27	AA08	AAA	78	0.160
A	C27 C28	AA00	AAA	86	0.202
A	C28 A29	AA00	AAA	96	0.162
A	A29 G30	AA00	AAA	79	0.206
A	G30 A31	AA00	AAA	64	0.333
A	A31 OMC32	AA08	AAA	81	0.179
A	OMC32 U33	AA00	AAA	74	0.262
A	U33 OMG34	OP04	OPN	46	0.181
A	OMG34 A35	AA08	AAA	80	0.245
A	A35 A36	AA00	AAA	58	0.462
A	A36 YYG37	AA00	AAA	63	0.267
A	YYG37 A38	AA00	AAA	35	0.336
A	A38 PSU39	AA08	AAA	91	0.223
A	PSU39 5MC40	AA00	AAA	85	0.245
A	5MC40 U41	AA00	AAA	80	0.211
A	U41 G42	AA08	AAA	93	0.185
A	G42 G43	AA00	AAA	90	0.150
A	G43 A44	AA00	AAA	82	0.201
A	A44 G45	AA00	AAA	44	0.440
A	G45 7MG46	NANT	NAN	0	0.748
A	7MG46 U47	NANT	NAN	0	0.660

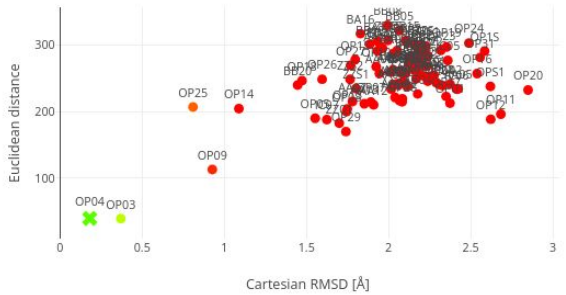
 How to c

(Computed) ▾ Add Rename Delete

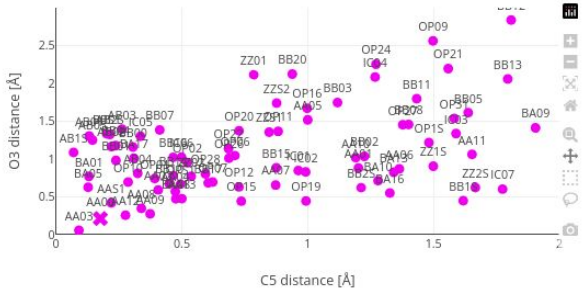
(Add your own NtC sets if you want to change the automatically assigned NtCs)

● - NtC ✕ - Currently shown NtC ■ - Computed NtC

Similarity plot



Connectivity to previous step



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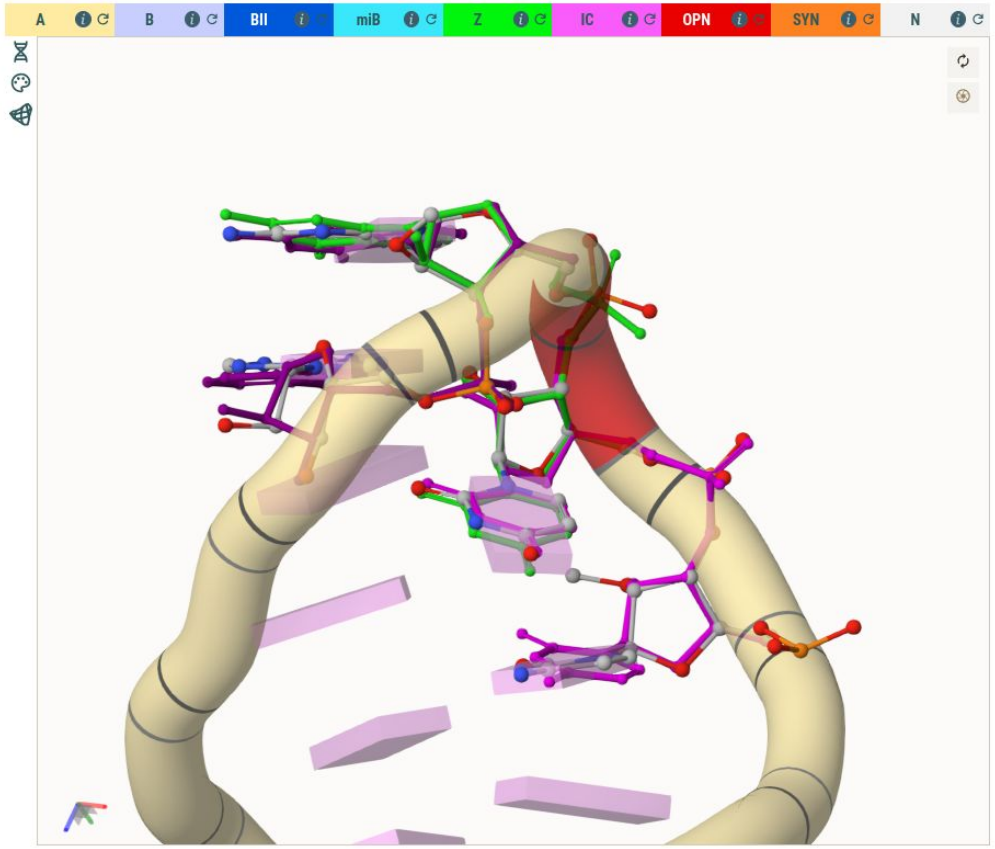
A B BII miB Z IC OPN SYN N



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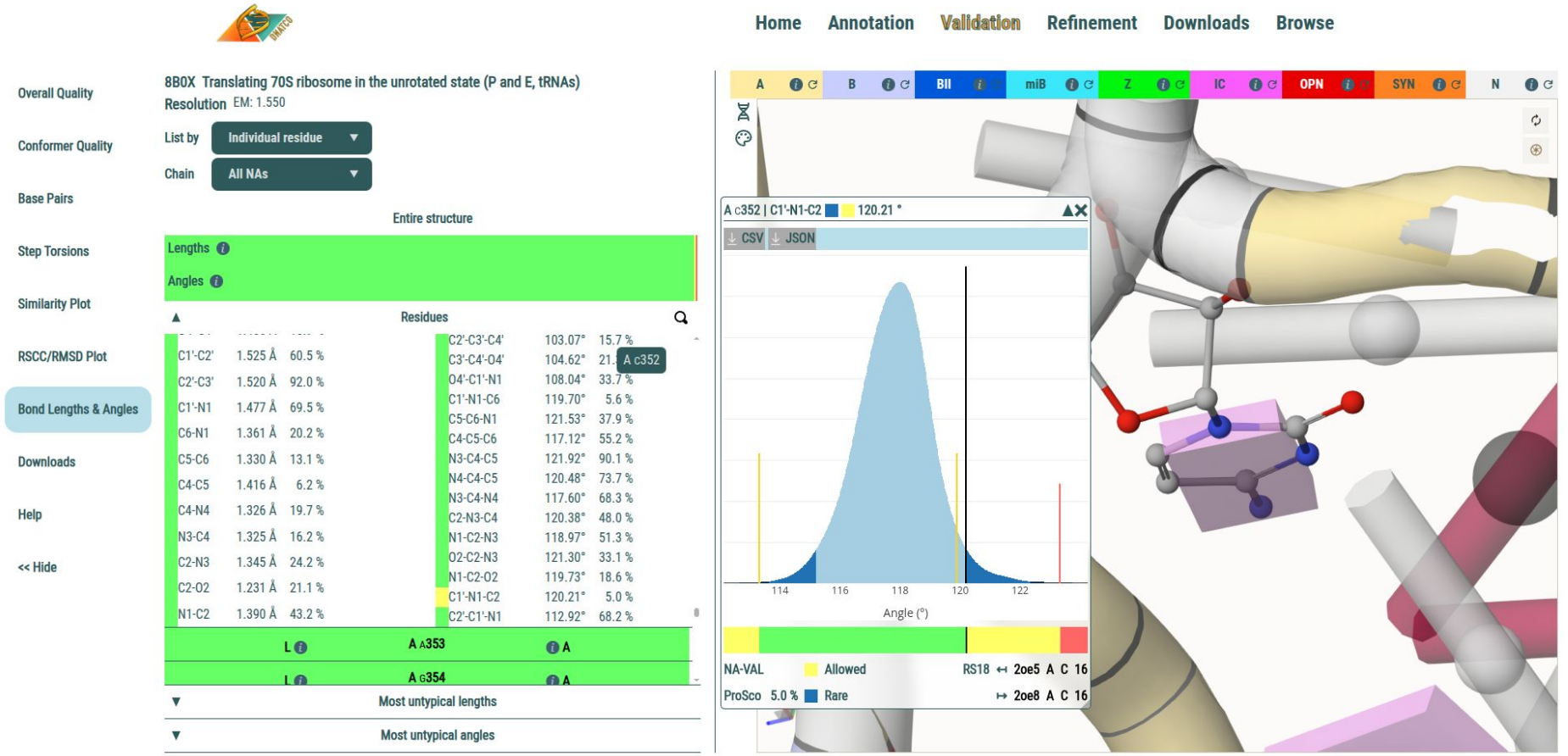
(NA-VAL) valence geometry validation



Černý J, Nicholls RA, Brzezinski D, Berman HM, Gilski M, Joosten RP, Kowiel M, Lawson CL, Moriarty NW, Richardson JS, Schneider B, Vonrhein C, Williams CJ, Jaskólski M, Egli M. “New targets and procedures for validating the valence geometry of nucleic acid structures.” *Nucleic Acids Res.* ***2026***, https://doi.org/10.1093/nar/gkaf1335 - also https://github.com/cernylab/libnaval

(NA-VAL) valence geometry validation, whole PDB

NA type	Method	Bonds			Angles		
		Count	Of Concern (%)	Apr2024 PDB outliers (%)	Count	Of Concern (%)*	Apr2024 PDB outliers (%)
DNA	X-ray	8.1M	0.5	0.3	12.5M	0.7	0.8
	cryoEM	9.0M	0.5	0.2	13.9M	0.8	0.8
	NMR	5.0M	2.2	1.4	7.6M	4.7	4.2
RNA	X-ray	92.0M	0.2	0.1	143.5M	0.5	0.5
	cryoEM	132.5M	0.6	0.3	206.6M	0.6	0.6
	NMR	6.2M	0.9	0.5	9.6M	2.3	2.6

* About 0.1% “Of Concern” would be expected for a good structure

Černý J, Nicholls RA, Brzezinski D, Berman HM, Gilski M, Joosten RP, Kowiel M, Lawson CL, Moriarty NW, Richardson JS, Schneider B, Vonrhein C, Williams CJ, Jaskólski M, Egli M. “New targets and procedures for validating the valence geometry of nucleic acid structures.” *Nucleic Acids Res.* ***2026***, https://doi.org/10.1093/nar/gkaf1335 - also https://github.com/cernylab/libnaval

DNATCO provides

web application
- interactive tables, graphs, and Mol* visualization
- https://dnatco.datmos.org

standalone (Node.js) version
- multi-platform
- all functions (CLI, no GUI)
- will be included in CCP4 10
- https://github.com/cernylab/dnatco/releases

mmCIF for
- backbone conformations
  - with sugar puckers
- pairing (and unpaired)

CSV/JSON/text
- bond lengths and angles validation
- refinement restraints for REFMAC, Servalcat, Phenix, Coot, Buster
- commands for MMB (re)building
- Reference Sets

PDF
- full validation report

Complete source codes at https://github.com/cernylab

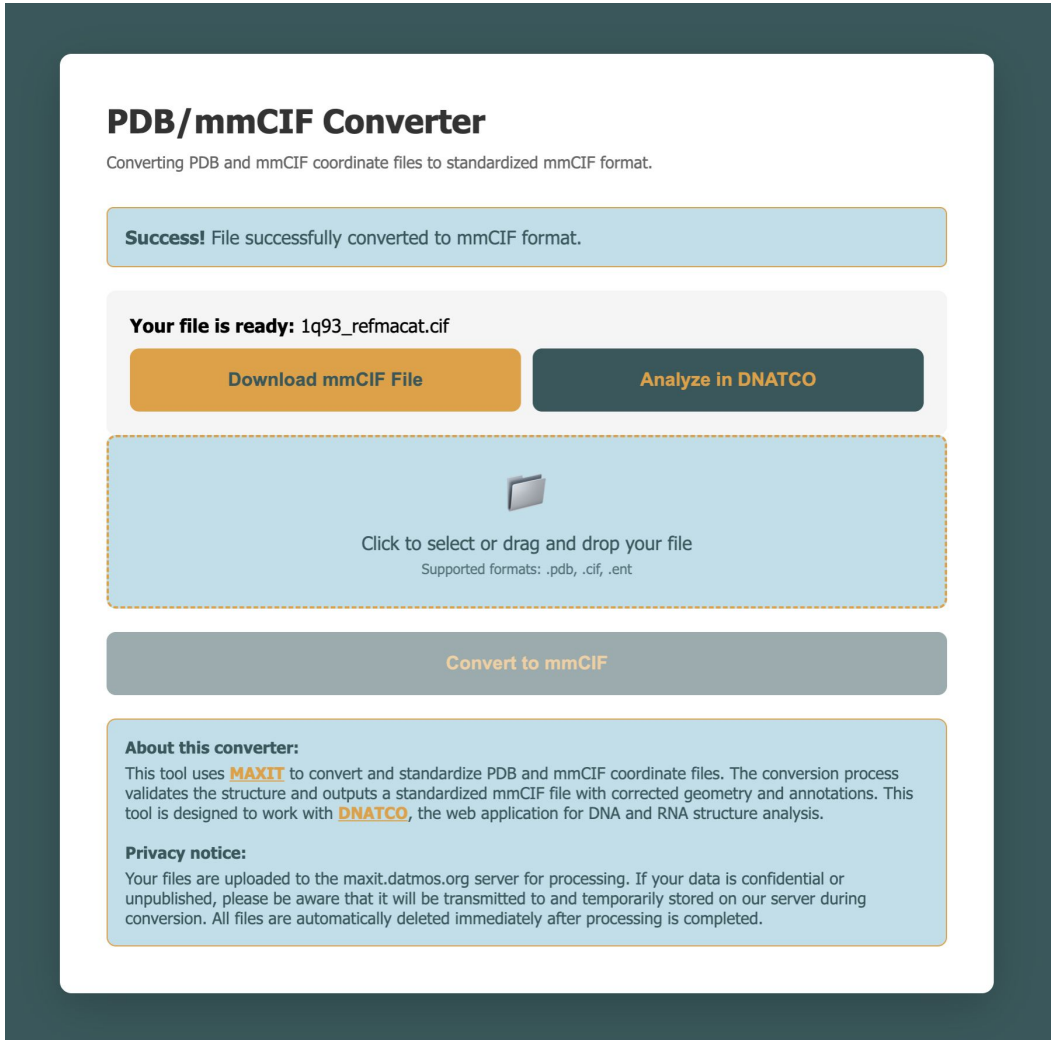
more tools

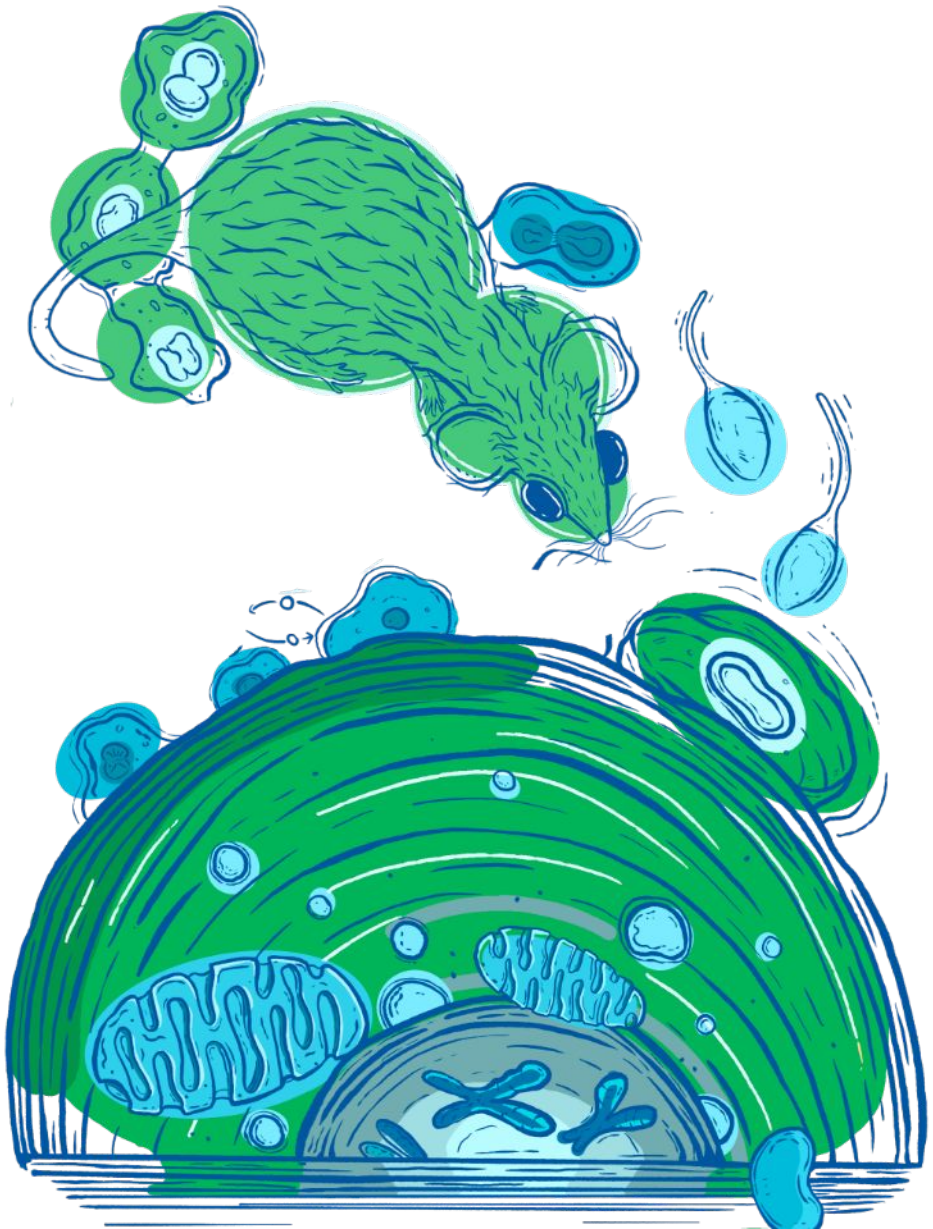
DNATCO Nextflow pipeline

- outcome of NA Hackathon 2026
- most of the DNATCO functions, container/grid/cloud ready
- nextflow run cernylab/dnatco-nf
- Linux/Mac/Windows(WSL) with docker/podman/container
- github.com/cernylab/dnatco-nf

MAXIT

- PDB↔mmCIF conversion
- https://maxit.datmos.org
- linked to DNATCO





DNATCO team

Paulína Božíková
Michal Malý
Jakub Svoboda
Terezie Prchalová
Daniel Šrom
Lada Biedermannová
Bohdan Schneider

DNATCO mmCIF

We developed a DNATCO-specific mmCIF dictionary extension in 2020 and since then we are using mmCIF files as the primary data resource.

- collaboration with Brinda Vallat was essential and made the whole process feel simple
- any software reading mmCIF gets transparently access to the DNATCO data
- dictionary is available at http://mmcif.rcsb.org/dictionaries/mmcif_ndb_ntc.dic/Index

```
_ndb_struct_ntc_overall.entry_id  1EHZ
_ndb_struct_ntc_overall.confal_score 61.8
_ndb_struct_ntc_overall.confal_percentile 81
_ndb_struct_ntc_overall.ntc_version 3.5
_ndb_struct_ntc_overall.cana_version 2.3
_ndb_struct_ntc_overall.num_steps 75
_ndb_struct_ntc_overall.num_classified 62
_ndb_struct_ntc_overall.num_unclassified 13
_ndb_struct_ntc_overall.num_unclassified_rmsd_close 0

loop_
_ndb_struct_ntc_step_summary.step_id
_ndb_struct_ntc_step_summary.assigned_CANA
_ndb_struct_ntc_step_summary.assigned_NtC
_ndb_struct_ntc_step_summary.confal_score
_ndb_struct_ntc_step_summary.euclidean_distance_NtC_ideal
_ndb_struct_ntc_step_summary.cartesian_rmsd_closest_NtC_representative
_ndb_struct_ntc_step_summary.closest_CANA
_ndb_struct_ntc_step_summary.closest_NtC
_ndb_struct_ntc_step_summary.closest_step_golden
1  AAA AA00 91 16.1  0.174 AAA AA00 1nzg_B_DG_13_DT_14
2  AAA AA00 91 15.1  0.161 AAA AA00 2vuq_A_U_4_U_5
3  AAA AA00 83 19.8  0.172 AAA AA00 4o41_A_G_104_C_105
4  AAA AA00 74 22.2  0.206 AAA AA00 370d_B_DC_11_DG_12
5  AAA AA08 93 17.7  0.163 AAA AA08 1vq8_0_U_967_G_968
6  A-B AB05 71 21.4  0.205 A-B AB05 1j9h_A_U_2_G_3
7  OPN OP11 52 50.3  0.455 OPN OP11 4arc_B_A_7_U_8
8  NAN NANT 0  83.2  0.899 ICL IC02 4v88_A6_U_58_C_59
```

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Work in progress

- Restraints for X-ray and cryoEM refinement
  - REFMAC/Servalcat, Buster, Phenix, Coot
- Enhanced sampling MD in gromacs
  - PMF-based enhanced sampling MD
  - tens of ns superior to μs classical MD
- Modeling and density fitting
  - MMB (MacroMoleculeBuilder)
  - webMMB
  - Coot
  - Moorhen