



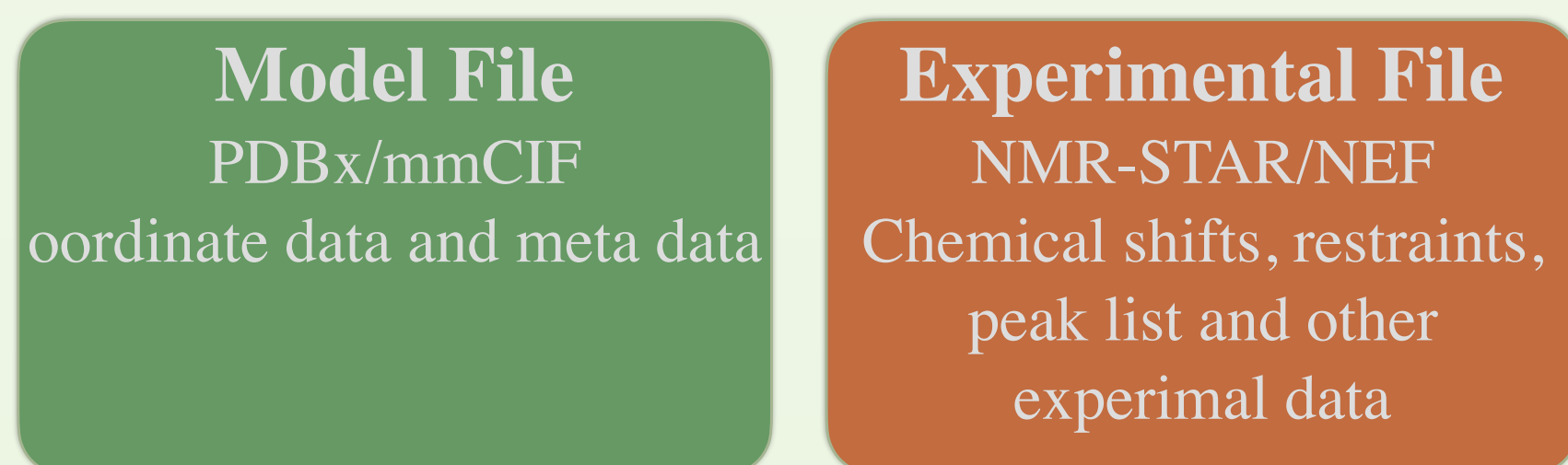
No more PDB format files! Welcome to PDBx/mmCIF ecosystem

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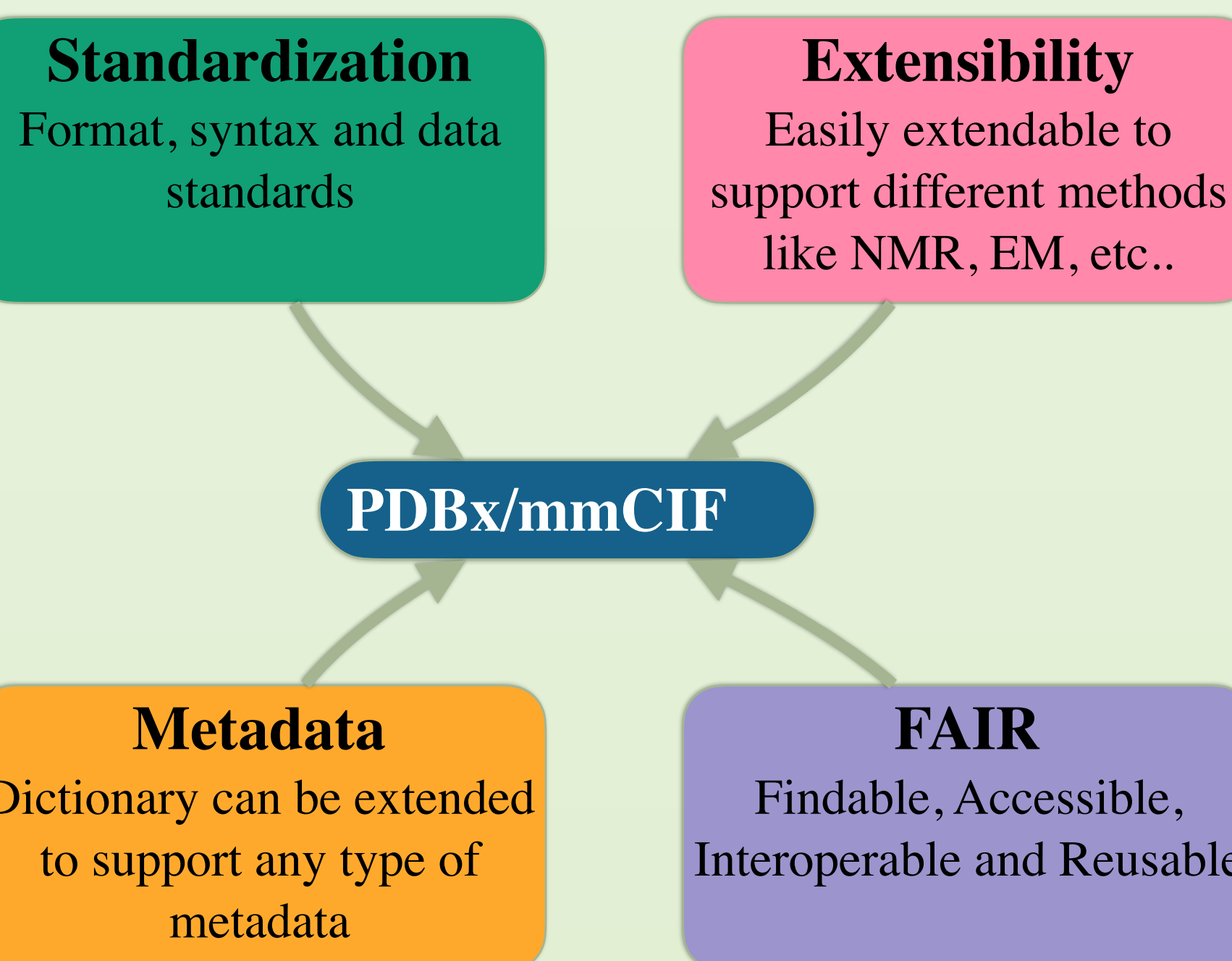
wwPDB data deposition



wwPDB accept data coming from structure determination studies whereas BMRB accepts all kids of NMR data including raw experimental data.

PDBx/mmCIF Format

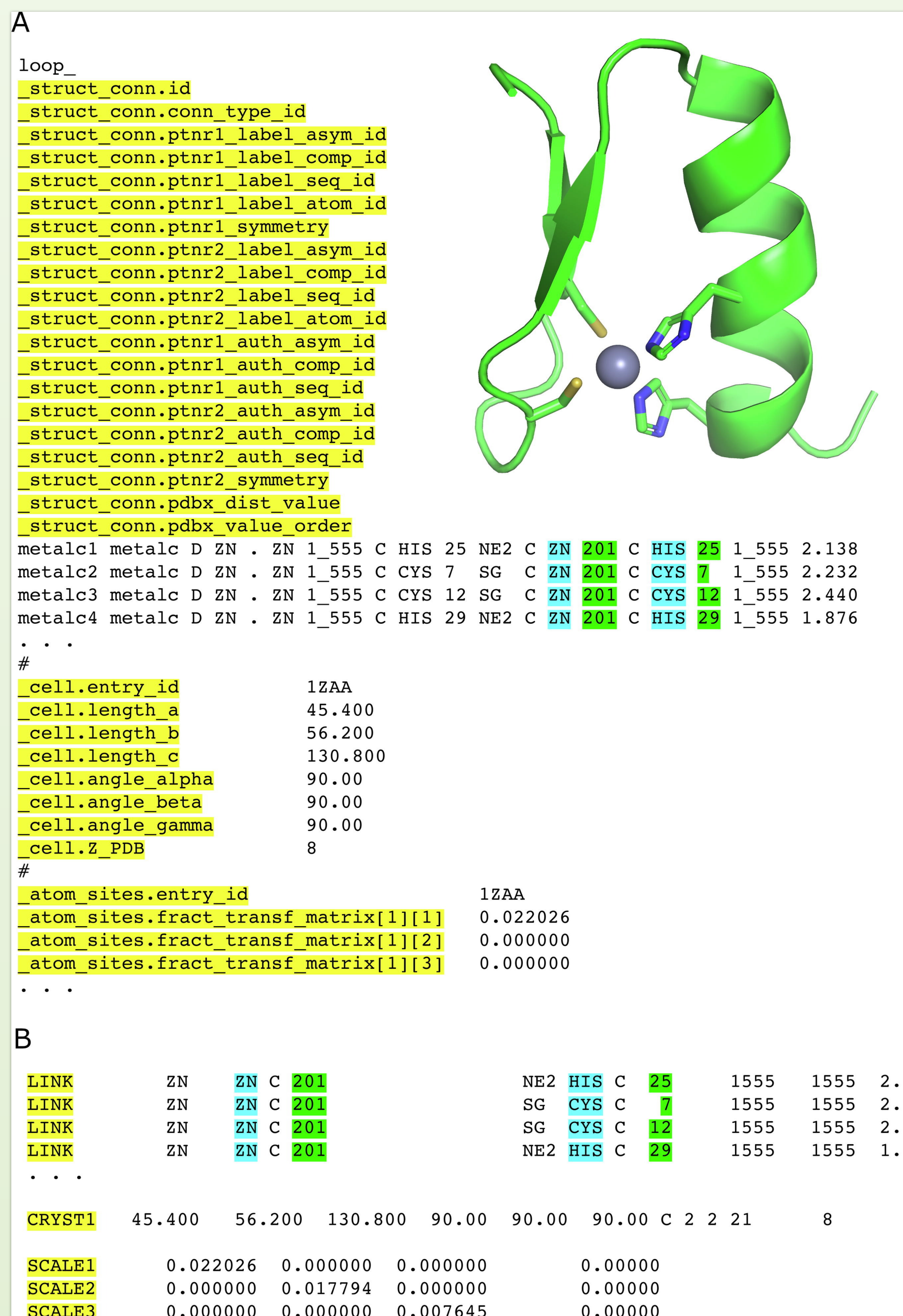
PDBx(Protein Data Bank exchange)/mmCIF(macromolecular Crystallographic Information File) is the master archival format of the PDB since 2014



Limitations of legacy PDB format

- Fixed size columns
- Column informations hard coded
- Limited scope for meta data
- Can't be used represent large molecules like viruses
- No support to define biological assemblies
- No way define ligand interaction
- No way to define ensemble properties
- No way to represent conformers

Metadata



(A) Partial PDBx/mmCIF file for PDB ID 1ZAA. N.B.: Every data value has a key and multiple rows of data may be described in a table. The yellow highlighting describes the category and attributes. For the _struct_conn category, green depicts the residue numbers and cyan the component type. (B) Equivalent metadata records in legacy PDB format. Similar color coding depicts the mapping between category keys and record names as in (A), with LINK records highlighting the residue number and cyan the chemical component type. Inset figure, one of the zinc finger domains in 1ZAA depicting the sidechains that interact with the bound zinc ion codified in (A) and (B).

PDBx/mmCIF Resource

- Dictionary resource <https://mmcif.wwpdb.org/>
- Virtual crash course <https://pdb101.rcsb.org/train/training-events/mmcif>
- Create your mmCIF <https://pdb-extract.wwpdb.org/>
- Software resource <https://mmcif.wwpdb.org/docs/software-resources.html>

NMR-STAR data model

NMR-STAR is the archival format for NMR data at wwPDB and BMRB.



NMR-STAR Resource

- Dictionary resource <https://bmr.io/dictionary/>
- Parser <https://pypi.org/project/pynmrstar/>
- Data visualization <https://pypi.org/project/pybmr/>

Why PDBx/mmCIF and NMR-STAR?

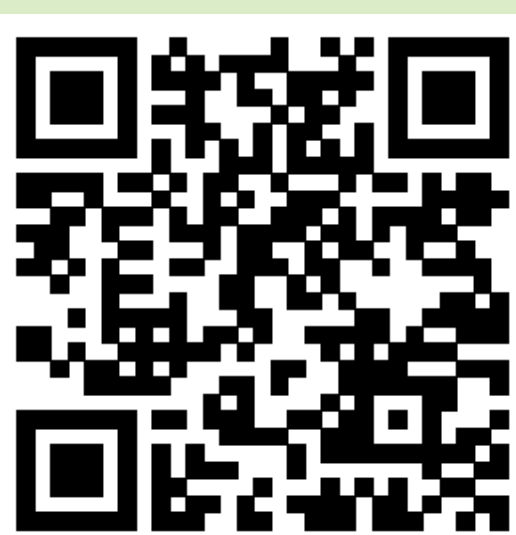
Integrative and hybrid methods have become more common and model files are required to carry the necessary meta data from different experiments in addition to the coordinate information. The complexity of the information like multiple conformations, ligand interactions, screening studies require proper data modeling with can only be possible using PDBx/mmCIF and NMR-STAR.

Join Us!

If you are a software developer and your software is capable of generating model data and NMR data then join us as an NMR mmCIF working group member and contribute to the data modeling and software development.

Contact: help@bmr.io

- Westbrook, *et al.*, (2022) PDBx/mmCIF Ecosystem: Foundational Semantic Tools for Structural Biology *JMB* 434: 167599 doi: [10.1016/j.jmb.2022.167599](https://doi.org/10.1016/j.jmb.2022.167599)
- Ulrich, *et al.* NMR-STAR: comprehensive ontology for representing, archiving and exchanging data from nuclear magnetic resonance spectroscopic experiments. *J Biomol NMR* 73, 5–9 (2019). doi: [10.1007/s10858-018-0220-3](https://doi.org/10.1007/s10858-018-0220-3)



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