Structural Bioinformatics Training Workshop & Hackathon 2018

mmtfPyspark Datastructures

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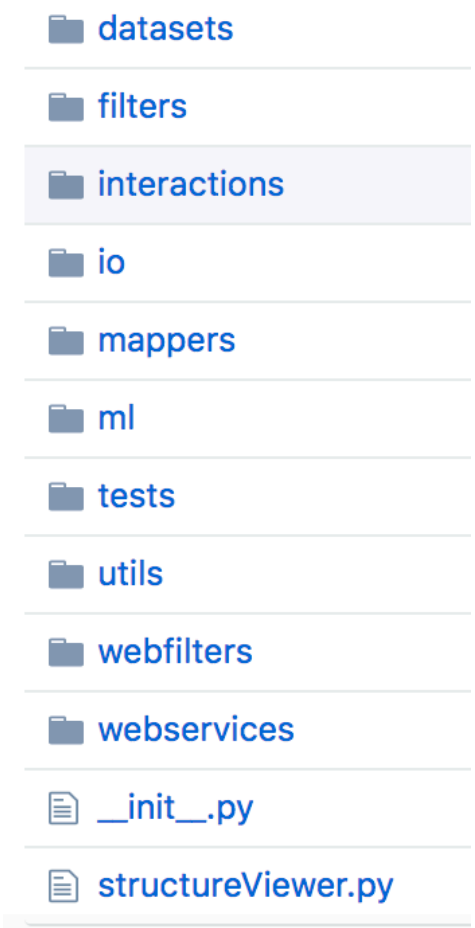
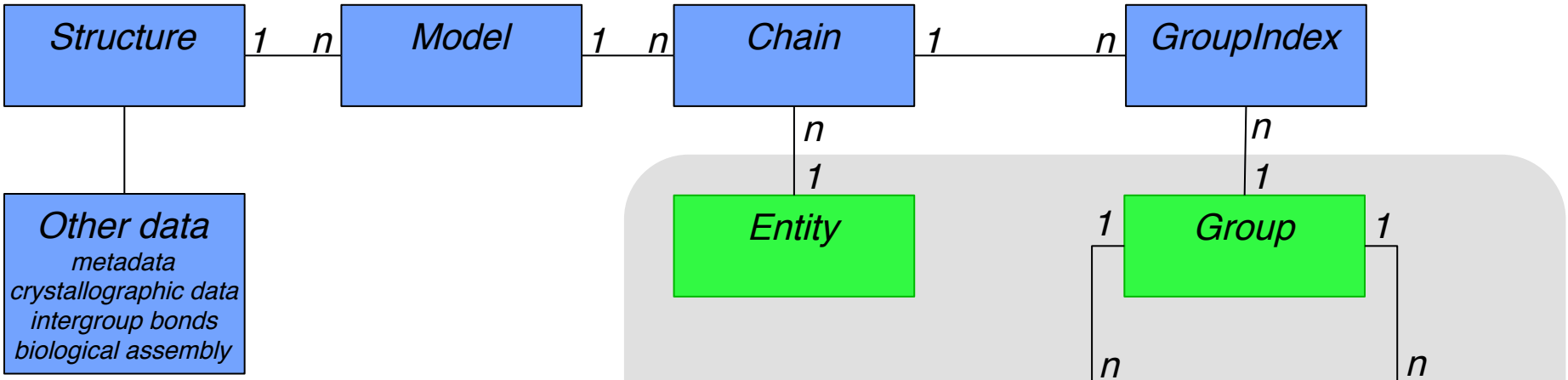
mmtfPyspark Modules Covered



- **utils**
  - Core mmtf data structures
  - Misc. utility methods

MMTF Datastructure

Flat (columnar encoded) data structure with an implicit hierarchy



Entity
A unique molecule in a structure, e.g., polymer chain, ligand, or water

Group
A unique chemical group (residue)

unique entities and groups are stored only once
e.g., 20 natural amino acids, water

Columnar Datastructure

- Atom-array-based datastructure as numpy arrays
- Enables efficient operations, including boolean indexing
- Chain and group indices are available
  - Chain to atom indices
    - Index to first atom in chain
    - Index to last atom in chain + 1
  - Chain to group indices
    - Index to first group in chain
    - Index to last group in chain + 1
  - Groups to atom indices
    - Index to first atom in group
    - Index to last atom of group + 1

Jupyter Notebook Tutorials

- 1-MMTF-Datastructure
- 2-ColumnarDatastructure
- 3-ColumnarStructureIndexing
- Problem-1 (Solution-1)
- Problem-2 (Solution-2)

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