

APBS 2.0

v.1 - hello world - unit testing infrastructure

v.2 - pdb2pqr integration

- new data structure - read in a file (registering)

- breaking apart Routines.py

v.3 - integrate APBS calls

- pqr plugin file

- call APBS - multigrid elect

→ clean repository

Do do:

repo ✓

create env

- boot strapper

req - py3

- numpy

- unit test something

planned framework

implement framework

- (on file data (hand coded))

- plugin loader

basic plugin interface