**PDB Projects Journal**

**UPDATE: Map PDB structures to their genomic coordinates:**

1. Place all PDB structures into a single directory
2. Update pdb.config with the necessary information
   1. If the database does not yet exist or you want to overwrite the existing, then set create\_new\_db to True
   2. If you do not want pdbmap.py to find human homologues for non-human PDB structures, set disable\_human\_homologue to False
3. Run `pdbmap.py -c pdb.config`

**Download PDB Structure(s):**

1. Download PDB from RCSB – Step 2 to batch download from a list of PDB IDs
2. Paste PDB IDs into <http://www.rcsb.org/pdb/download/download.do>
   1. Check PDB Format
   2. Select uncompressed
   3. Download all files

**Generate PDB Annotation File from MySQL:**

1. Open the MySQL database containing PDB information
2. Select columns: *pdbid,chain,seqres,x,y,z,chr,start,end*
3. Save to space delimited file
4. In RVCLUST
   1. Load *rvclustobject* with PEDMAP information
   2. *rvobj <- annotate(rvobj,”PDB”,c(“PDB\_x”,”PDB\_y”,”PDB\_z”))*
   3. May also choose to use *PDBID, CHAIN*, or *SEQRES* for labeling or clustering

**Compute SDP Scores and Load Candidate PDB Structures:**

1. Feed FASTA file to group\_sim\_sdp.py
   1. This generates the SDP scores
2. Feed the SDP score output to fasta\_to\_pdb.py
   1. This loads the SDP scores into the database
3. Feed FASTA file to pull\_unp.py
   1. Pulls all uniprot IDs in the FASTA file
4. Download all relevant PDB structures
   1. PDB\_query\_by\_unp.xml has a REST template for pulling PDB IDs by UNP
   2. Manually: <http://www.rcsb.org/pdb/software/wsreport.do>
   3. Automatically, learn how to script an “XML Post”
   4. Use this list to download the relevant PDB structures
5. Feed PDB structures to pdbmap.py

**PyMol Visualization**

**Generate a PDB Cluster Map from RVCLUST**

1. Run the cluster analysis
2. Write the variants table to tab-delimited file with columns (in order): *pdbid,chain,seqres,value*
3. Open PyMol and fetch pdbid
4. In the cmd bar: *run overwrite\_pymol.py*
5. In the cmd bar: *overwrite\_bfactors(‘pdbid’,’tab-delim from step 3’)*

**Generate a PDB Map from in MySQL:**

1. Open the MySQL database containing PDB information and SDP values
2. Join as necessary and select columns (in order): *pdbid,chain,seqres,value*
3. Save to tab delimited file
4. Open PyMol and fetch pdbid
5. In the cmd bar: *run overwrite\_pymol.py*
6. In the cmd bar: *overwrite\_bfactors(‘pdbid’,’tab-delim from step 3’)*

**Rotate 360 degrees x axis, Rotate 360 degrees y axis Movie**

1. orient
2. mset 1 x360
3. movie.roll 1,180,1,axis=y
4. movie.roll 181,360,1,axis=x
5. mplay
6. orient;mset 1 x360; movie.roll 1,180,1,axis=y; movie.roll 181,360,1,axis=x;