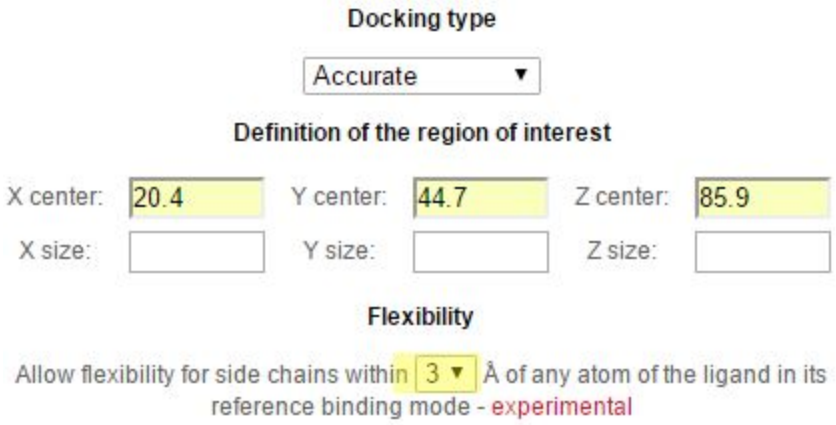
Step 3.3 - Place the ligand into the protein

1. Go to http://www.swissdock.ch/docking
2. In the target selection, upload the file "<PDB>_relaxed.pdb"
3. In the ligand selection, upload the "LIG.pdb" file created in the prev step. **BUT** - make sure to upload it in MOL2 format. How to save LIG.pdb as LIG.mol2:
   a. Open chimera
   b. Open LIG.pdb file
   c. Click file -> save MOL2

   Then upload the LIG.mol2 file to the site.
4. Enter description and email address
5. Click on "show extra parameters" and edit the options. You should see the following:



6. Wait for mail with the results….
7. Open mail and go to results page. Download the results by clicking the icon

8. Get a zip file. Unzip it and then untar it. (just run the commands:)

   ```
   unzip <zip file name>
   tar xf complexes.tar.xz
   ```
9. Get your desired result (usually will be complex0_0) and open it in chimera. In chimera do:
   a. Select ->structure -> ligand
   b. Select -> Invert (selected models)
   c. Action -> Atoms/bonds -> delete
   d. Save as "LIG_positioned.pdb"
10. Open "LIG_positioned.pdb" in text editor and make sure it look something like that:
    Note: in every row it should be LIG X and not LIG A or any other thing… and try to not

add extra spaces as it messes the pdb file.

```
HETATM    4  O1  LIG X   1      20.275  42.930  84.368  1.00  0.00           O
HETATM    5  C3  LIG X   1      20.374  45.621  83.764  1.00  0.00           C
HETATM    6  C4  LIG X   1      20.502  45.266  82.280  1.00  0.00           C
HETATM    7  O2  LIG X   1      19.757  45.934  81.513  1.00  0.00           O
HETATM    8  O3  LIG X   1      21.390  44.421  81.988  1.00  0.00           O
HETATM    9  O4  LIG X   1      22.193  42.940  85.588  1.00  0.00           O
HETATM   10  H1  LIG X   1      23.030  45.107  83.384  1.00  0.00           H
```