Exercise 5

Bio.PDB numpy and Pymol

We are working with trypsin again. The exercise is to pull away the inhibitor from the enzyme, rotate it, and alter the b-factor of the atoms in the inhibitor. Each part is visualised using Pymol. The direction should be directly away form the enzyme, and the distance 20 Ångstrøm. The rotation is a 90º counterclockwise rotation around the direction the inhibitor was moved.

Move the I chain

5.0
Open the pdb structure using Bio.PDB

5.1
Make two numpy arrays containing the atom positions for chain E and I. Only include atoms from residues containing a Cα atom

5.2
Use the previous arrays to calculate the center of the two chains, and the direction from the E chain to the I chain (a direction has unit length). Record the direction.

5.3
Move the I chain 20 ångström in the direction you just calculated.

5.4
Write the structure to a pdb file and investigate the result in Pymol. Save an image in a representation of your choice.

Rotate the I chain

5.5
Use the supplied rotation matrix to rotate the inhibitor around its own centre. Remember that a rotation matrix rotates around the origin of the coordinate system. The rotation matrix, R, is used by premultiplying it to a point.

$$x_{rotated} = R \cdot x$$

5.6
Save the structure and check the rotation using Pymol

Modify the B-factors of the I chain

5.7
The b-factors are easily accessible from Pymol and can be used to colour the structure. Alter the b-factor of the I chain according to the following formula. Save the structure

$$b = \cos\left(\frac{2\pi i}{100}\right) \cdot 20 + 25$$

where *i* is an atom index for chain I.

5.8
Open the structure in Pymol and colour the structure according to b-factor, record an image. Try action->preset->b factor putty
Describe the result.

Hints
- atom.get_coord() gives you a numpy array
- atom.get_vector() gives you a Bio.PDB.Vector object (this has some special properties e.g., minus is overloaded to give the distance between two atoms)
- See if a residue has a Cα atom with res.has_id('CA')
- numpy arrays have a method called mean
- The x-coordinate of the direction is 0.1188 Å