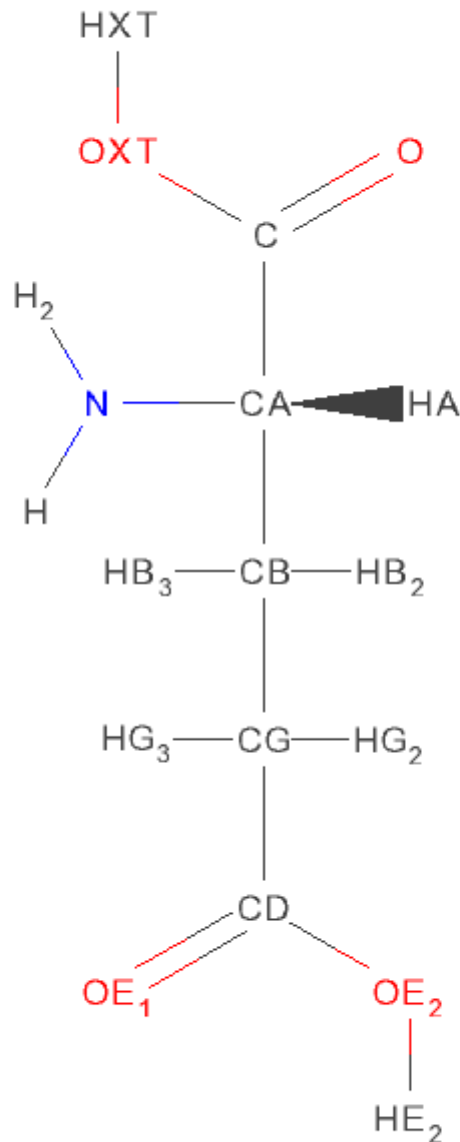


# How to add rotamer making rules to parameter file?

If a residue or a cofactor has rotatable single bond, the user needs to define the rotation rule so that MCCE can make rotamers accordingly.

In MCCE, the rotation is for heavy (non H) atoms only, and H atoms have their own position optimization rules.



Let's look at glutamic acid (GLU). Its backbone atoms N, C, CA are considered "fixed". The side chain atoms CB, CG, CD, OE1 and OE2 are susceptible to rotation. Here is how the rotation rules are defined in glu.ftpl file.

```
# Rotatable bonds. The atoms extended in the bond direction will all be rotated.
ROTATE, GLU: " CA " - " CB ", " CB " - " CG ", " CG " - " CD "
```

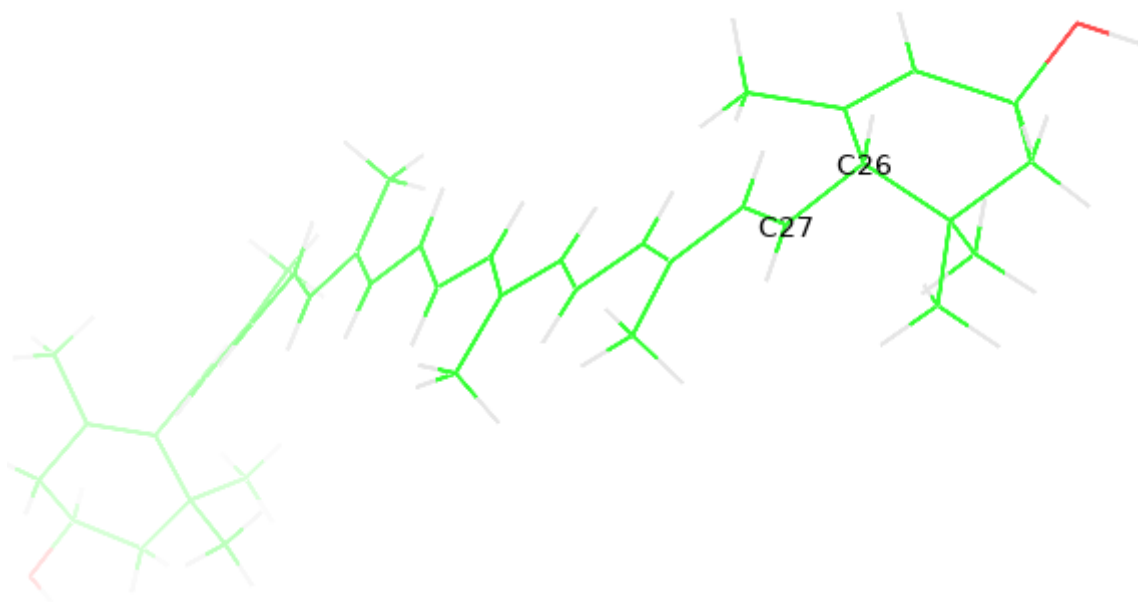
The first part, which is before ":" sign, is the parameter key "ROTATE, GLU". It means this line is rotation rule for GLU residue.

The second part, which is after ":" sign, is the parameter value " CA " - " CB ", " CB " - " CG ", " CG " - " CD ". The atom names are in quotes because the atom names in PDB format are 4-char

including spaces. The parameter value defines 3 rotatable bonds, and each rotatable bond is defined by two atoms.

- The order of two atoms that define a rotatable bond is important. Follow the direction of the first atom to the second atom, all atoms connected to the second atoms will rotate around this rotatable bond.
- The order of rotatable bonds does not matter in MCCE rotamer making.
- The rotations resulted from multiple rotatable bonds are stackable, which means, rotations around one bond will be build on the rotations around another bond.
- All rotation rules of the same residue must be defined in a single ROTATE parameter line.

Lets look at another molecule LUT. In this molecule, all heavy atoms are either in conjugated double bond system or contrained by the ring except the bond between C26 and C27. C26 is  $sp^3$  hybrid orbital that breaks the conjugated double bonds, so C26 and C27 bond is only rotatable bond.



Since there are more atoms on the C27 side, I assume the C27 side atoms are "fixed" and C26 atoms are susceptible to rotation. Therefore this ROTATE line would be a good start in its ftpl file

```
ROTATE, LUT: " C27" - " C26"
```

After putting this line in ftple file and rerun step 2, I get the following result:

```
step2.py -l 2
$ cat rot_stat
```

Rotamer making statistics:

Residue	Start	Clean	Swap	Rotate	Self	Hbond	Repack	Ioni.	TorH	OH	Elect
LUTs1620	1	1	1	4	1	1	1	1	2	9	2
Total	1	1	1	4	1	1	1	1	2	9	2

MCCE created 3 additional rotamers in the middle of step 2, but they were ruled out due to the high self energy of these new rotamers.

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Revision #3

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