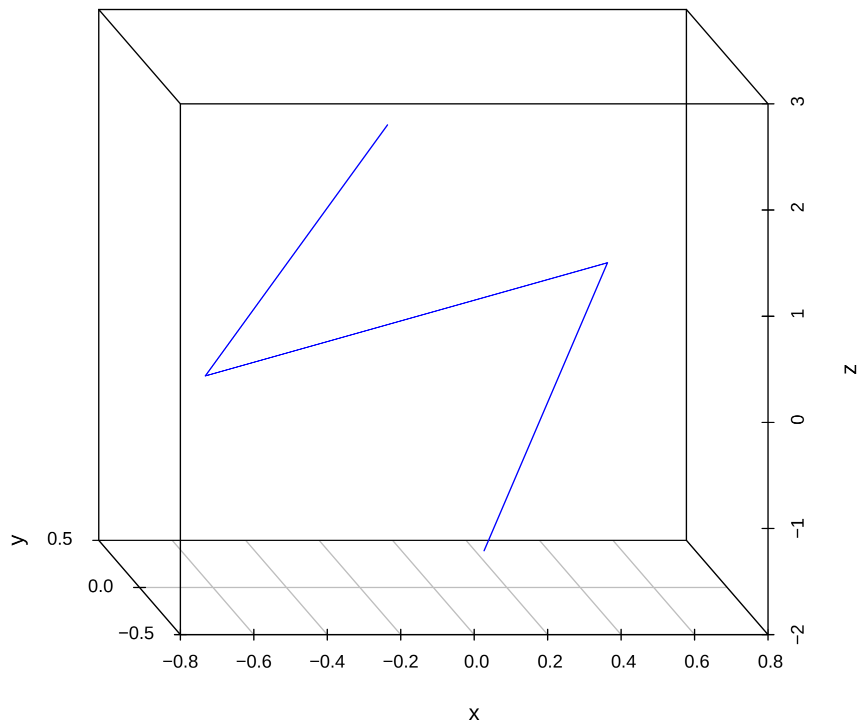
The beginning coordinates of the dihedral are:

$$S\ (0.138, 0.0, -1.654)$$
$$C_1\ (0.474, 0.0, 1.059)$$
$$C_2\ (-0.621, 0.0, -0.007)$$
$$O\ (-0.125, 0.0, 2.357)$$

When plotted this looks like this:



We want to rotate the 4th atom O about the dihedral axis which is defined by the $C - C$ vector. This means the vector and the axis of rotation are:

$$\text{axis} = \vec{a} = \vec{C}_2 - \vec{C}_1 = (-0.621 - 0.474, 0.0 - 0.0, -0.007 - 1.059) = (-1.095, 0.0, -1.066)$$
$$\text{vector} = \vec{v} = \vec{O} - \vec{C}_2 = (-1.25 + 0.621, 0.0 - 0.0, 2.357 + 0.007) = (-0.629, 0.0, 2.364)$$
$$\text{angle of rotation} = \theta = \frac{\pi}{2}$$

The quaternion operator that defines this operation is (from Quaternions and Spatial Rotations - Wikipedia):

$$
\begin{aligned}
\vec{q} &= \cos(\frac{\pi}{4}) + \sin(\frac{\pi}{4}) \cdot \frac{1}{\|\vec{a}\|}\vec{a} \\
\|\vec{a}\| &= \sqrt{(-1.095)^2 + 0^2 + (-1.066)^2} = 2.446 \\
\vec{q} &= \frac{1}{\sqrt{2}} + \frac{1}{2.446\sqrt{2}}(-0.629, 0.0, 2.364) = \frac{1}{\sqrt{2}}(1 + (-0.257,\ 0.0,\ 0.966377))
\end{aligned}
$$

In addition we need the inverse which is obtained by just reversing the signs of the imaginary components:

$$
\vec{q}^{\ -1} = \frac{1}{\sqrt{2}}(1 + (0.257,\ -0.0,\ -0.966377))
$$

The rotated vector is then:

$$\vec{v}_{new} = \vec{q}(\vec{a})\vec{q}^{\,-1}$$

$$\vec{q}(\vec{a})\vec{q}^{\,-1} = (a_0 + a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k})(0 + v_1\mathbf{i} + v_2\mathbf{j} + v_3\mathbf{k})(a_0 - a_1\mathbf{i} - a_2\mathbf{j} - a_3\mathbf{k})$$
$$=(a_0(v_1\mathbf{i} + v_2\mathbf{j} + v_3\mathbf{k}) + a_1(-v_1 + v_2\mathbf{k} - v_3\mathbf{j}) + a_2(-v_1\mathbf{k} - v_2 + v_3\mathbf{i}) + a_3(v_1\mathbf{j} - v_2\mathbf{i} - v_3))*$$
$$(a_0 - a_1\mathbf{i} - a_2\mathbf{j} - a_3\mathbf{k})$$
$$=((-a_1v_1 - a_2v_2 - a_3v_3) + (a_0v_1 + a_2v_3 - a_3v_2)\mathbf{i} + (a_0v_2 - a_1v_3 + a_3v_1)\mathbf{j} + (a_0v_3 + a_1v_2 - a_2v_1)\mathbf{k})*$$
$$(a_0 - a_1\mathbf{i} - a_2\mathbf{j} - a_3\mathbf{k})$$

Going term by term we get:

$$(-a_1v_1 - a_2v_2 - a_3v_3) = (-(-0.18173 * -0.629) - (0.0 * 0.0) - (0.683332 * 2.364)) = -1.7297$$
$$(a_0v_1 + a_2v_3 - a_3v_2)\mathbf{i} = (\frac{1}{\sqrt{2}} * (-0.629) + (0.0 * 2.364) - (0.68333 * 0.0))\mathbf{i} = -0.445\mathbf{i}$$
$$(a_0v_2 - a_1v_3 + a_3v_1)\mathbf{j} = (\frac{1}{\sqrt{2}} * 0 - (-0.18173 * 2.364) + (0.68333 * -0.629))\mathbf{j} = -0.00021\mathbf{j}$$
$$(a_0v_3 + a_1v_2 - a_2v_1)\mathbf{k} = (\frac{1}{\sqrt{2}} * 2.364 + (-0.18173 * 0) - (0 * -0.629))\mathbf{k} = 1.6716\mathbf{k}$$

Putting this back in the original equation we get:

$$\vec{v}_{new} = (x_0 + x_1\mathbf{i} + x_2\mathbf{j} + x_3\mathbf{k}) * (a_0 - a_1\mathbf{i} - a_2\mathbf{j} - a_3\mathbf{k})$$

Applying the last multiplication we get:

$$((x_0 * a_0) - (x_1 * -a_1) - (x_2 * -a_2) - (x_3 * -a_3))+$$
$$((x_0 * -a_1) + (x_1 * a_0) + (x_2 * -a_3) - (x_3 * -a_2))\mathbf{i}+$$
$$((x_0 * -a_2) - (x_1 * -a_3) + (x_2 * a_0) + (x_3 * -a_1))\mathbf{j}+$$
$$((x_0 * -a_3) + (x_1 * -a_2) - (x_2 * -a_1) + (x_3 * a_0))\mathbf{k}$$