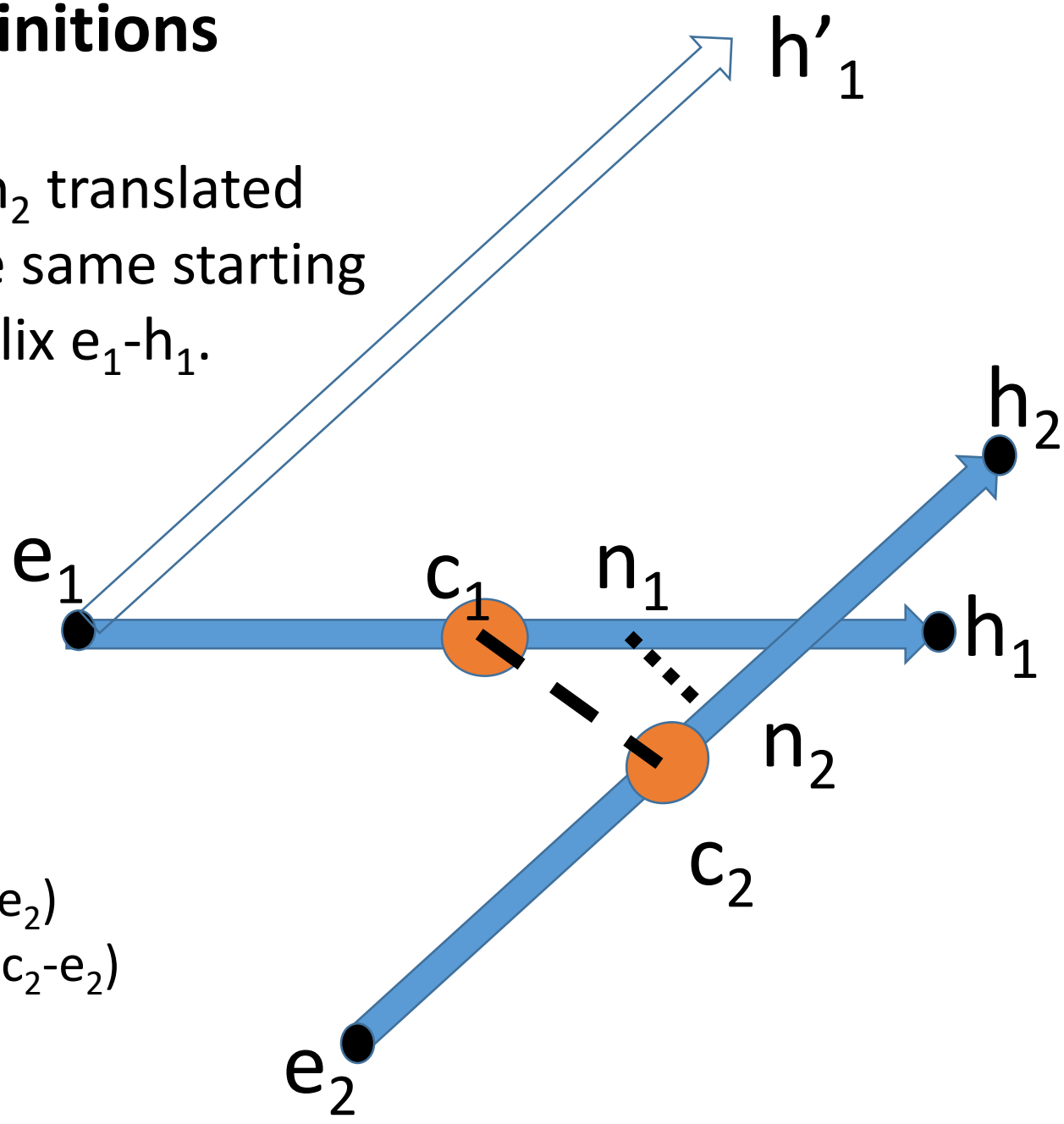
Helix-helix distance and angle definitions

c_1, c_2: centers of helices 1 and 2, resp.

The dotted line connecting n_1 and $n_2$is the shortest connecting helices 1 and 2. The angles e_1-n_1-n_2 and e_2-n_2-n_1 are both 90°.

h'_1 is helix e_2-h_2 translated to have the same starting point as helix e_1-h_1.



$$cc\_dist = \|\overrightarrow{c_1} - \overrightarrow{c_2}\|$$

$$dist = \|\overrightarrow{n_1} - \overrightarrow{n_2}\|$$

$$dee1 = \|\overrightarrow{e_1} - \overrightarrow{e_2}\|$$

$$dee2 = \|\overrightarrow{h_1} - \overrightarrow{e_2}\|$$

angle=ang(h'_2-e_1-h_1)

dhang=tors(e_1-n_1-n_2-e_2)

*dhang*_cc=tors(e_1-c_1-c_2-e_2)

Helix-helix rotation definitions

$C\beta_{ir\_rep}$ is the β carbon of the residue that defines the HX-HX rotation, p is the site nearest to the $C\beta_{ir\_rep}$ on HX_1 axis, p' is 1Å away from p on the HX_1 axis and the c'_2-p' line is parallel to the line connecting c_2 with the point nearest to in on HX_1.

HX_1 rotation wrt HX_2 is the torsion angle defined by centers $C\beta_{ir\_rep}$ – p – p' - c'_2.