

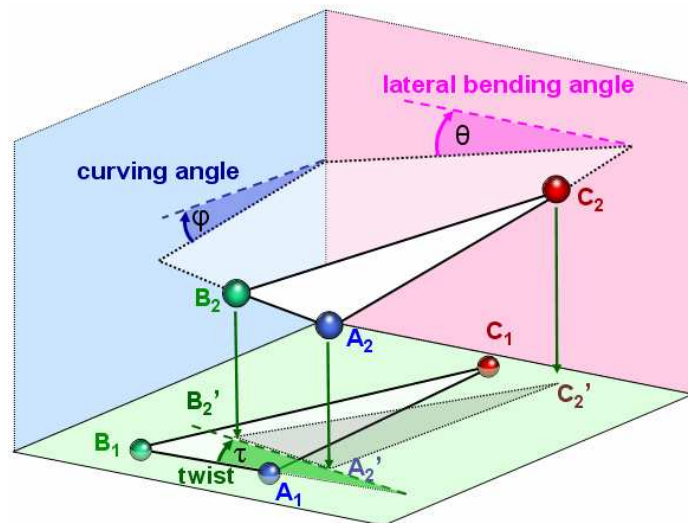
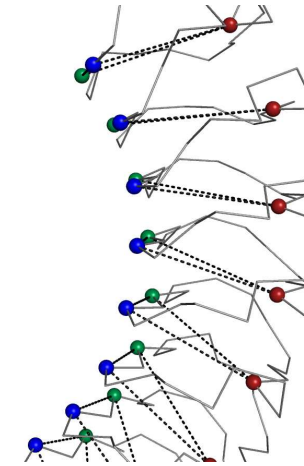
How does it work?

ANGULATOR provides a standardized description of the LRR-geometry, taking into account the interdependence of the three, rotation angles - curvature, twist and lateral bending - required to describe the overall geometry.

The orientation of each repeat is calculated only with respect to the preceding repeat, allowing the calculation of each angle independent of other geometric parameters.

For this purpose, we represent each LRR by a defined triangle based on three invariant atoms (A, B and C) per repeat.

As the β -strand on the concave side of LRR proteins is the most conserved structural feature of each repeat, the C_{α} -carbon atoms of residues at either end of the β -strand are chosen as points A and B. The outer, convex side of the LRR is more variable. Here, we chose the C_{α} -atom of a conserved hydrophobic residue across from the β -sheet as atom C (Pos. 15 in 21-residue repeats, pos. 16 in 20- or 22-residue repeats).



To simplify the geometric description, we define three mutually perpendicular planes for each pair of LRRs: The basal plane (green) incorporates the reference triangle $A_1-B_1-C_1$ representing the first LRR of each LRR-pair. The lateral plane (pink) is perpendicular to the basal plane (or $A_1-B_1-C_1$) and parallel to the vector A_1-B_1 . The facial plane (blue) is perpendicular to both $A_1-B_1-C_1$ and A_1-B_1 .

Geometrically, the twist τ of a particular LRR ($A_2-B_2-C_2$) with respect to its predecessor ($A_1-B_1-C_1$) is thus simply the angle between A_1-B_1 and $A_2'-B_2'$ - the projection of A_2-B_2 onto the basal plane (green angle).

The curving angle ϕ of $A_2-B_2-C_2$ relative to $A_1-B_1-C_1$, causing the overall horseshoe shape of the LRR-domain, is the angle of the projection of $A_2-B_2-C_2$ in the facial (blue) plane relative to the basal plane (blue angle).

Similarly, the lateral bending angle θ is the angle between the component of $A_2-B_2-C_2$ in the lateral (pink) plane relative to that of the basal plane (pink angle).