

- Clash analysis:
 - Align each conformation to the binding pocket and check if the linker region has steric clashes with the binding target.

- Cluster analysis:
 - Separate trajectory conformations into clusters to obtain the structural ensemble.

Simulation results are analyzed in two ways

Background

Project Description

Results

Conclusion

linker region has sterically clashed with the binding target.

Align each information to the binding packet and check if the

Cluster analysis:

Separate trajectory information into clusters to obtain the

• Clash analysis:

structural ensemble.

Crash Analysis