

Positional Disorder

This example will show you how to split atoms when there is a positional disorder.

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1. Run a refinement.
2. Split the C4, C9, C10 CF₃ groups.
3. Edit the file, remove the RIGU command.
4. Add H atoms and refine.
5. Refine anisotropically.
6. Refine the split F atoms isotropically.
7. Introduce third disorder positions for the F atoms on C10.
8. Apply distance restraints.
9. Refine.
10. Impose RIGU restraint.
11. Refine.