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ADVANCED SASSIE-WEB

TORSION ANGLE MONTE CARLO

- ▶ More extensible framework
- ▶ Input requires PSF (contains more physics)
- ▶ Currently available move sets:
 - ▶ Protein Backbone Dihedral
 - ▶ Single-Stranded Nucleic Acid Backbone Dihedral
 - ▶ B-Form Deoxyribonucleic Acid Bead–Rod
 - ▶ Isopeptide Bond Dihedral

FLEXIBLE AND POST INPUT

- ▶ [HIV-1 Gag matrix protein](#)
- ▶ Repeat changing "move direction" to `reverse`



FLEXIBLE AND POST INPUT

▶ Linear DNA Example



HANDS ON LEARNING

▶ Exercises

