**Identify the start and end residue numbers for each chain**

# Import necessary modules from BioPython

from Bio.PDB.PDBParser import PDBParser

import Bio.PDB.PDBIO

# Function to parse the .gro file and print residue ranges for each chain

def print\_residue\_ranges(file\_path):

# Since BioPython doesn't directly read .gro files, you'll need to convert it to a .pdb file

# Usually this would be done outside of Python, as BioPython does not handle .gro files natively

# For the purpose of demonstration, we're assuming 'file\_path' is a PDB file path here

parser = PDBParser(QUIET=True) # QUIET=True to avoid warnings about the PDB structure

structure = parser.get\_structure('MD\_system', file\_path)

for model in structure:

for chain in model:

residues = list(chain.get\_residues())

first\_residue = residues[0].get\_id()[1]

last\_residue = residues[-1].get\_id()[1]

print(f"Chain {chain.id}: Residue range {first\_residue} to {last\_residue}")

# Usage example, replace 'your\_structure.pdb' with your actual file path

print\_residue\_ranges('/Users/josephsteward/Downloads/5brz (1).pdb')

Chain A: Residue range 1 to 409

Chain B: Residue range 0 to 201

Chain C: Residue range 1 to 101

Chain D: Residue range 2 to 202

Chain E: Residue range 3 to 406