

Protein Repair and Analysis Server: A Web Server to Repair PDB Structures, Add Missing Heavy Atoms and Hydrogen Atoms, and Assign Secondary Structures by Amide Interactions

Osita Sunday Nnyigide, Tochukwu Olunna Nnyigide, Sun-Gu Lee* and Kyu Hyun*

School of Chemical and Biomolecular Engineering, Pusan National University, Busan 46241, Korea

*Correspondence to kyuhyun@pusan.ac.kr or sungulee@pusan.ac.kr

ABOUT CHAIN SELECTION

Users can specify a specific chain if they need to, otherwise all chains will be processed. The chain should be specified as a positive integer. PRAS will map the integer to alphabets. This is because a chain can start with any letter. Thus, 1 = the first chain, 2 = the second chain, 3 = the third chain, etc.

Note that if user makes an invalid selection (i.e., selecting a chain that does not exist in the file supplied) PRAS will notify user and then terminate the execution.

If user selects a specific chain, files generated from the assignment of secondary structure and plots of four Ramachandran types will be numbered 1 because there will be only one chain when the PRAS generated PDB or mmCIF structure is passed to these modules.