

Appendix B: Residue Parameter Files

Parameter files describing the chemical and structural properties of each residue is found in the PyRosetta package in the `minirosetta_database/chemical/residue_type_sets` directory.

The full-atom residue parameters are stored in the `/fa_standard/residue_types` directory. As an example, the parameter file for threonine is shown below.

```

NAME THR
IO_STRING THR T
TYPE POLYMER #residue type
AA THR
ATOM N Nbb NH1 -0.47
ATOM CA Cabb CT1 0.07
ATOM C CObb C 0.51
ATOM O OCbb O -0.51
ATOM CB CH1 CT1 0.14
ATOM OG1 OH OH1 -0.66
ATOM CG2 CH3 CT3 -0.27
ATOM H HNbb H 0.31
ATOM HG1 Hpol H 0.43
ATOM HA Hapo HB 0.09
ATOM HB Hapo HA 0.09
ATOM 1HG2 Hapo HA 0.09
ATOM 2HG2 Hapo HA 0.09
ATOM 3HG2 Hapo HA 0.09
LOWER_CONNECT N
UPPER_CONNECT C
BOND N CA
BOND N H
BOND CA C
BOND CA CB
BOND CA HA
BOND C O
BOND CB OG1
BOND CB CG2
BOND CB HB
BOND OG1 HG1
BOND CG2 1HG2
BOND CG2 2HG2
BOND CG2 3HG2
CHI 1 N CA CB OG1
CHI 2 CA CB OG1 HG1
PROTON_CHI 2 SAMPLES 3 60 -60 180 EXTRA 1 20

```

Residue identification information

PDB atom names, Rosetta atom types, and partial charges

Polymer connectivity information

Bond connectivity information

Defining side-chain torsion angles

Defining proton side-chain torsion angle sampling