Ring finding algorithm process with example variables:

Phase I – Locate rings

1. Find bonds by measuring all atom-atom distances
2. Delete all saturated carbons (carbons with >3 bonds)
3. Delete all carbon/heteroatoms with a coordination number <2
4. Repeat step 3 until there is no change in the number of atoms
5. Add all remaining atoms to both atom_array and atom_remaining_list
6. Select atom at random from atom_remaining_list (which is linked to atom_array)
7. Locate a chain of four carbon/hetero atoms bonded in a row from atom_array (gray label) append to temp_ring_array
8. Locate AngleA and AngleB for the *last* four items in temp_ring_array
9. If AngleA<AngleB, delete previous two atoms from temp_ring_array and search through different route (repeat step 7, but keeping two atoms)
    a. If AngleA<AngleB after multiple attempts, delete all gray labeled atoms (temp_ring_array) and start over (go to step 6)
10. If AngleA>AngleB, delete the *first* item in temp_ring_array, continue search (go to step 7)
11. For each atom added, repeat step 7-10 (for gray labeled atoms) until the fourth atom is found to be bonded to another ring or the search fails a preset number of times (step 9a)
12. If the ring is found, delete all ring atoms from atom_remaining_list and append ring atoms to global_ring_array.
13. Go to step 6
14. Halt process once atom_remaining_list is empty, or a pre-set number of attempts have failed to produce a ring

Phase II – Rotate rings and place Bqs

1. For each ring in global_ring_array:
    a. Select a random atom from first ring in global_ring_array
    b. Move random (or user chosen) atom to (0,0,0) coordinate
        i. Apply transformation to all XYZ coordinates
    c. Select a second random atom from first ring in global_ring_array
    d. Apply rotation to atom until it is in the XY plane
        i. Apply transformation to all XYZ coordinates
    e. Select a third random atom from first ring in global_ring_array
    f. Apply rotation to atom until it is in XY plane
        i. Apply transformation to all XYZ coordinates
    g. Locate ring centroid
        i. Place Bq at 1 angstrom (or user specified location) above ring

2. Remove previous ring from global_ring_array and repeat step 1 until there are no more rings.