Notes on XCrySDen

1. The view you get when you load a structure is the unit cell. The box drawn is the edge of the unit cell. An atom counts as inside the cell if its center is: we have to worry about sharing between cells only if the atom is exactly on the edge, face, or corner.
   Only atoms inside the unit cell are drawn, but atoms exactly on the boundaries or corners will be shown in multiple copies. The cell is in 2D, with only 2 lattice vectors.
2. Atoms are colored according to a default color for each element. You can change these if necessary if the atoms in your structure happen to have the same default color.
   Modify->Atomic Colors
3. XCrySDen draws bonds based on a simple distance criteria, using default atomic radii for each atom. Whether a line is drawn does not always correspond to the physical concept of bonds given the arbitrary cutoff. You can adjust these to make bonds show up if they don't, for ease of visualization.
   Modify->Atomic Radius. Increase the chemical connectivity factor a little and click "Update." Adjust so that the bonds you want appear and ones you don't do not appear.
4. You can expand beyond the unit cell to have multiple copies, helpful for judging what the crystal structure looks like on a bigger scale.
   Modify->Number of Units Drawn. The boxes shown are still the unit cell.
5. Rotating the system to view from different angles: click, hold down, and drag to rotate. You can align to different Cartesian directions with the buttons on the right that have red arrows.
6. To measure bond lengths: At the bottom of the pane, Distance button. Then click on the two atoms.
7. To measure bond angles: At the bottom of the pane, Angle button. Then click on the three atoms.
8. Note: You can determine properties of the lattice vectors by measuring lengths and angles between atoms that are periodic replicas of each other, i.e. constitute a lattice.
9. The coordinate system can be viewed by pressing the keyboard shortcut "y".