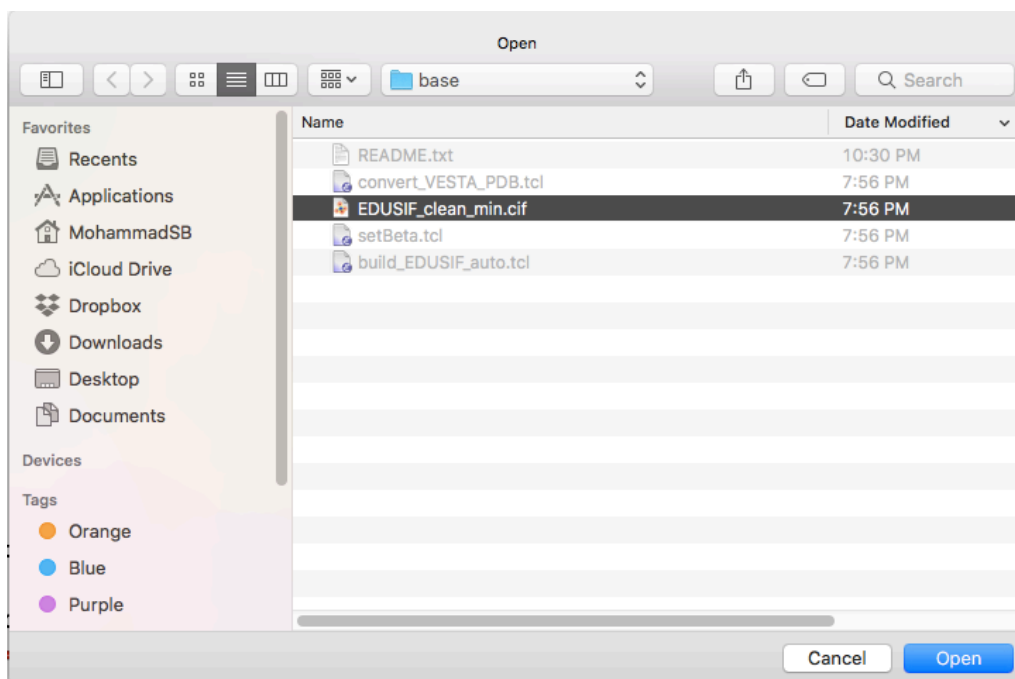
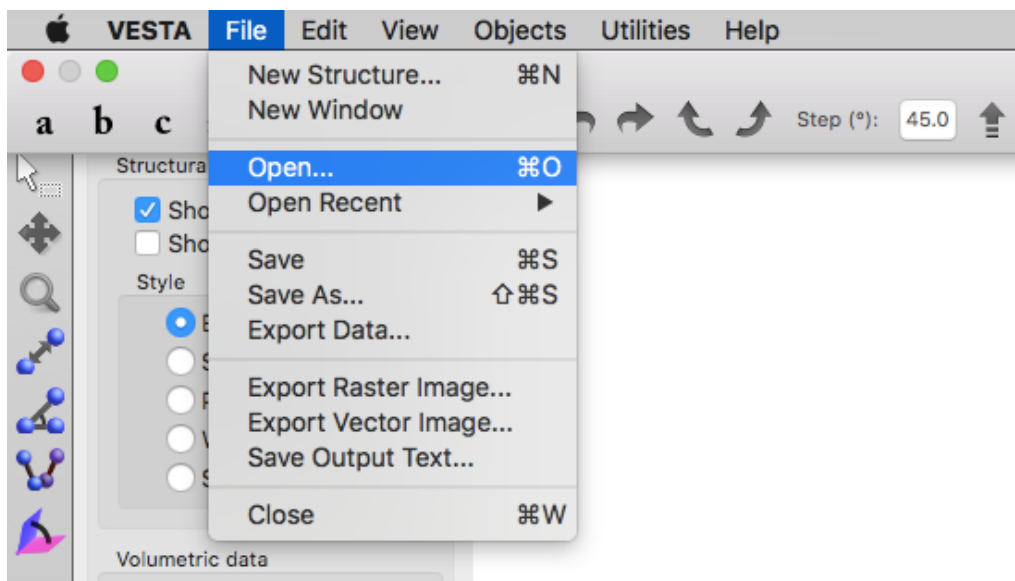


VESTA

VESTA is a 3D visualization program for structural models, volumetric data such as electron/nuclear densities, and crystal morphologies. VESTA has many novel features but here we use VESTA to visualize the cif file, extend the unit cell and export it as PDB file.

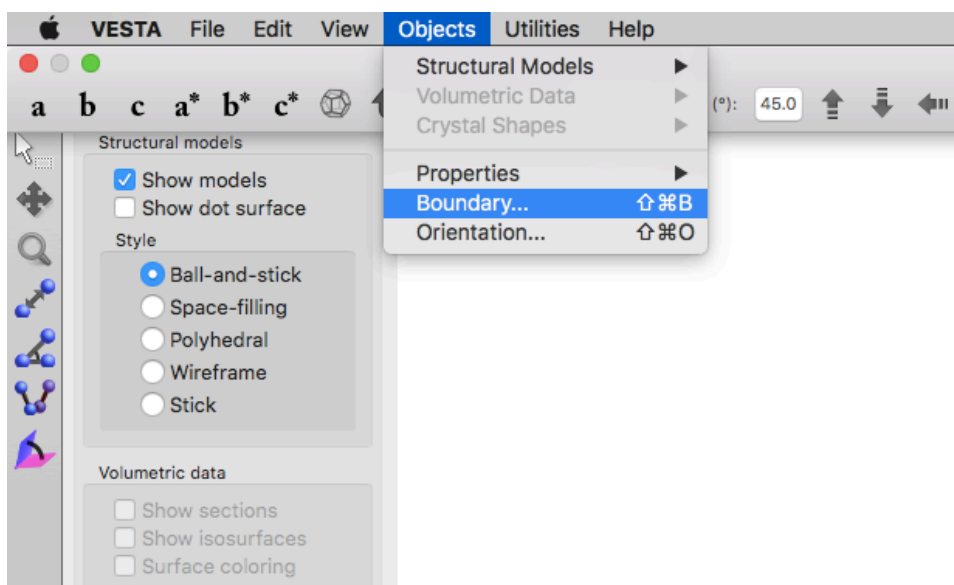
1. Load the structure (.cif)

Open the VESTA application. To load the new structure, we can drag and drop the structure on VESTA window or under “File” tab, click on “Open...” and open the “EDUSIF_clean_min.cif” file.

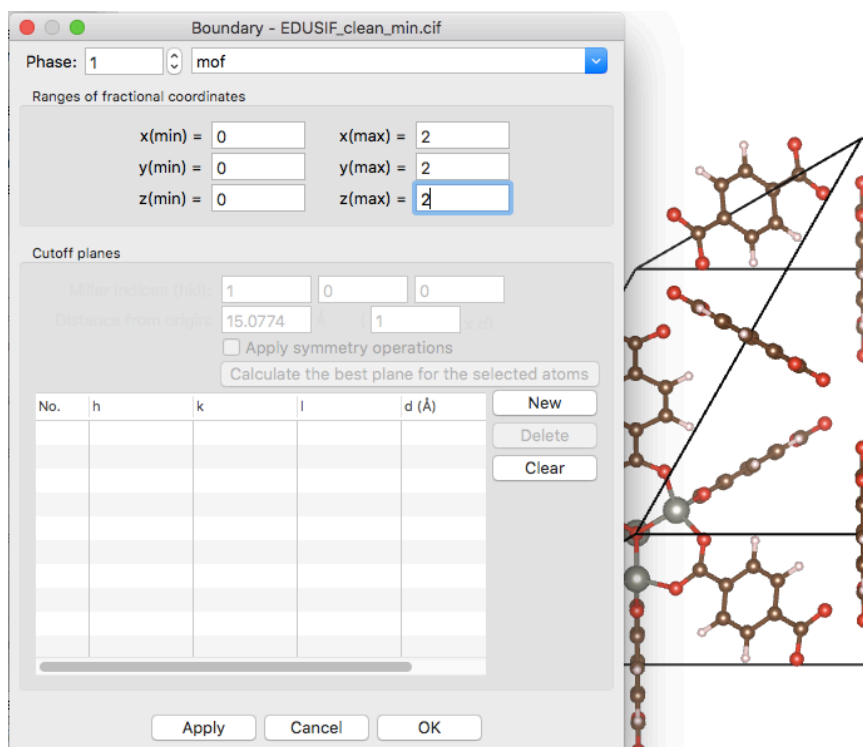


2. Extend the boundary

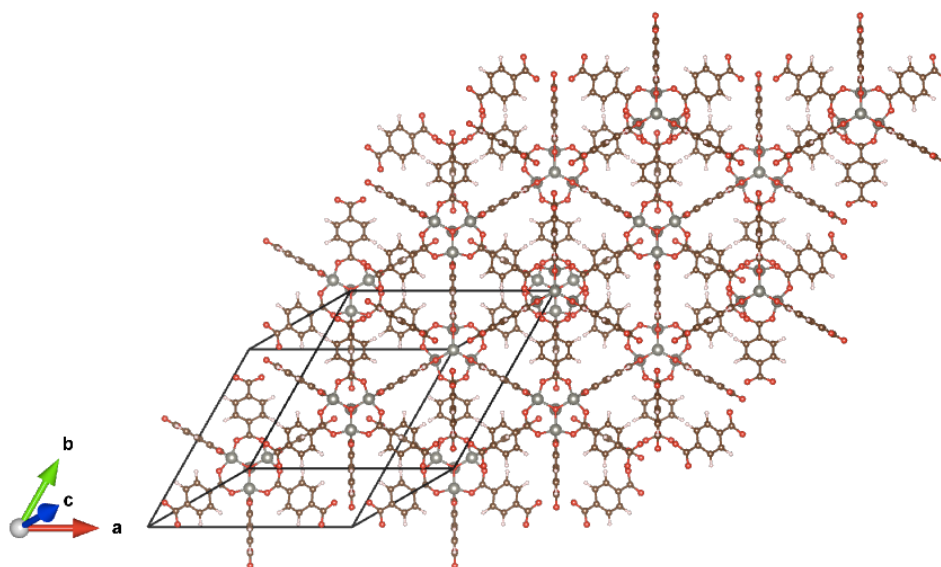
In order to extend the unit cell twice in x, y, and z direction, under “Objects” tab, select “Boundary...” to open “Boundary” window.



Change the value of x(max), y(max), and z(max) to 2. Then press OK.

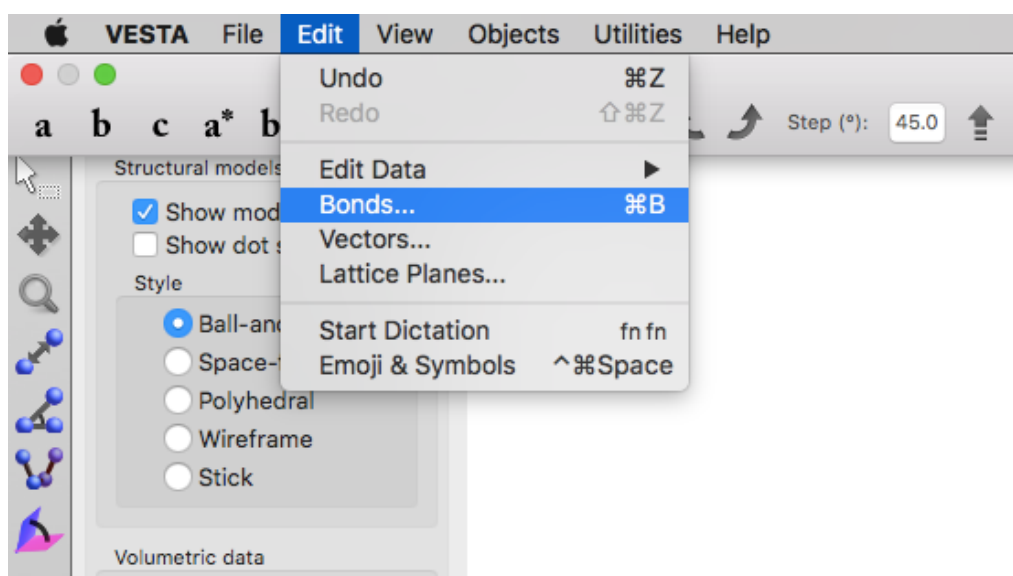


After unit cell extension, the IRMOF-1 structure should be like this:



3. Remove the extra atoms

One last step before export the structure to PDB is to remove the atoms that are not within the box. Under “Edit” tab, select “Bounds...” to open the “Bounds” window.



Bonds - EDUSIF_clean_min.cif

Phase: 1 mof

Search bonds and atoms

Search mode

- ☒ Search A2 bonded to A1
- ☐ Search atoms bonded to A1
- ☐ Search molecules

Boundary mode

- ☐ Do not search atoms beyond the boundary
- ☐ Search additional atoms if A1 is included in the boundary
- ☒ Search additional atoms recursively if either A1 or A2 is visible

☐ Search by label ☒ Show polyhedra

A1: C A2: O Min. length: 0 Max. length: 1.97249

No.	Atom 1	Atom 2	Min. (Å)	Max. (Å)	Bound.	Poly.	
1	C	O	0	1.97249	3	<input checked="" type="checkbox"/>	
2	C	C	0	1.89002	3	<input type="checkbox"/>	
3	C	H	0	1.2	2	<input type="checkbox"/>	
4	Zn	O	0	2.41693	2	<input checked="" type="checkbox"/>	

New Delete Clear

Apply Cancel OK

Select and delete every bound found in this section and click OK.

Bonds - EDUSIF_clean_min.cif

Phase: 1 mof

Search bonds and atoms

Search mode

- ☒ Search A2 bonded to A1
- ☐ Search atoms bonded to A1
- ☐ Search molecules

Boundary mode

- ☐ Do not search atoms beyond the boundary
- ☒ Search additional atoms if A1 is included in the boundary
- ☐ Search additional atoms recursively if either A1 or A2 is visible

☐ Search by label ☒ Show polyhedra

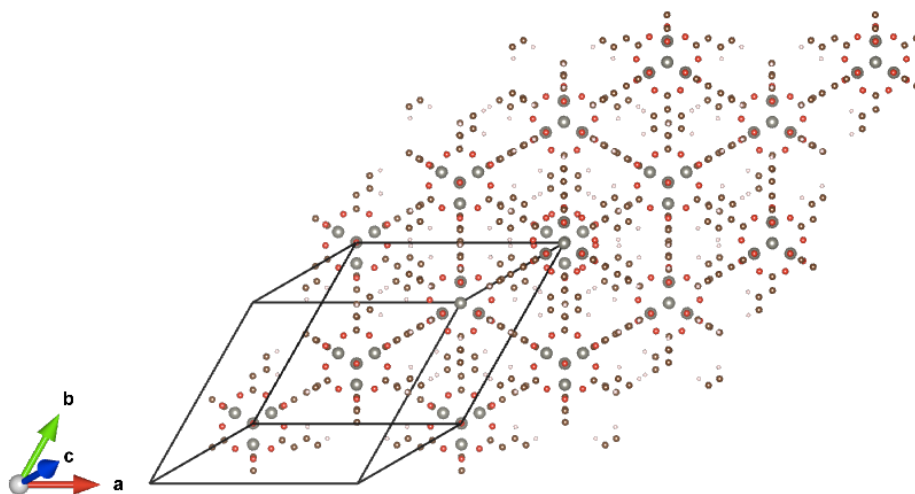
A1: Zn A2: O Min. length: 0 Max. length: 2.41693

No.	Atom 1	Atom 2	Min. (Å)	Max. (Å)	Bound.	Poly.	

New Delete Clear

Apply Cancel OK

After removing the bounds, the IRMOF-1 structure should be like this:



4. Export the structure as PDB

Last step is to export the structure into the PDB format. Under “File” tab, select “Export Data...”, and press “Save” button.

