**TUTORIAL EXPO: SOLUTION BY DIRECT METHODS**

The **Solution by Direct Methods** folder contains:

* **Example of default correct solution (Default folder)**
* **Example of correct solution obtained by exploring all the Direct Methods trials (Alltrials folder)**

**• Default folder**

It contains: **LaTi.exp** [the input file for the default run of *EXPO* in case of non-perovskite compound LaTi2Al9O19, after that the cell and the space group have been determined]; **LaTi.rtv** (the file containing the experimental profile counts); **LaTi\_true.cif** (the CIF file of the true model); **LaTi.pdf** (the file of the published structure).

The input file ‘LaTi.exp’ consists of the following lines:

%structure LaTi

%job LaTi

%data

cell 22.59355 10.99919 9.72968 90 98.5634 90

spacegroup C2/c

content (Al9LaO19Ti2)8

pattern LaTi.rtv

%continue

To run EXPO on LaTi in default way:

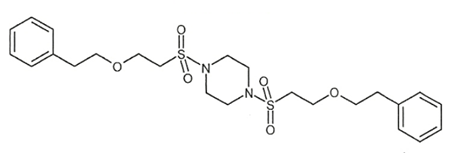
* Click on EXPO icon
* **File** in the upper Menu
* **Load & Go**
* Use ‘LaTi.exp’ as Input File and give the Output Filename you like (LaTi.out is the default output file name)
* **Go**
* **OK**
* Click on **Next** to go on continuously until the end of the run.

The structure model obtained at the end of the Direct Methods procedure, executed on the first set of phases (default choice), is the correct one. All the 32 atoms in the asymmetric unit are correctly located.

The obtained solution can be compared with the published fractional coordinates contained in the LaTi\_true.cif file. It can be done by the graphic pathway described below (See **Comparison with an external model** paragraph).

**• Alltrials folder**

It contains: **piperazine.exp** [the input file for the default run of *EXPO* in case of 1,4-Bis-(2-phenethyloxy-ethanesulfonyl)-piperazine (C24H34N2O6S2), after that the cell and the space group have been determined]; **piperazine.pow** (the file containing the experimental profile counts); **piperazine.fra** (the file of the fractional coordinates and the isotropic thermal parameters of the true model, hydrogen atoms excluded); **piperazine.pdf** (the file of the structure information published in **paper.pdf)**.

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The input file ‘piperazine.exp’ consists of the following lines:

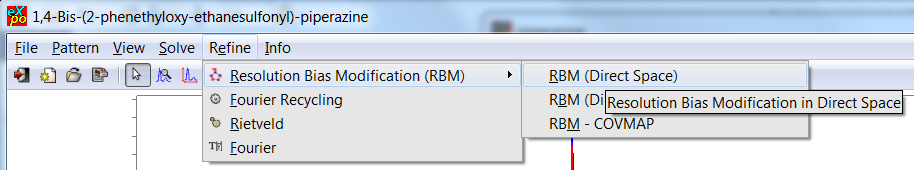
|  |
| --- |
| %Structure piperazine  %Job 1,4-Bis-(2-phenethyloxy-ethanesulfonyl)-piperazine  %Data  Cell 13.442 5.182 19.796 90 108.74 90  SpaceGroup p 21/a  Content (C24H34N2O6S2)2  Pattern piperazine.pow  %continue |

To run EXPO on piperazine in default way:

* Click on EXPO icon
* **File** in the upper Menu
* **Load & Go**
* Use ‘piperazine.exp’ as Input File and give the Output Filename you like (piperazine.out is the default output file name)
* **Go**
* **OK**
* Click on **Next** to go on continuously until the end of the run.

The structure model obtained at the end of the Direct Methods procedure, executed on the first set of phases (default choice), is not interpretable.

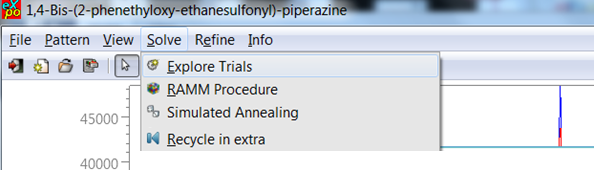
It is so rough and uninterpretable that is not advisable to try to improve it, for example, by cyclic application of RBM (RBM is advisable because the structure is organic). Indeed, by clicking on **Refine > Resolution Bias Modification (RBM) > RBM (Direct Space)** in the upper Menu,



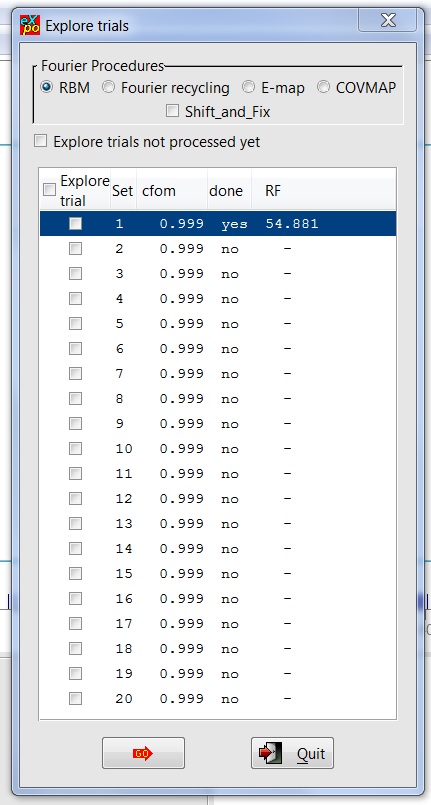
no improvement of the structure model is attained.

We can try to explore the other Direct Methods trials as follows:

**Solve > Explore Trials** in the upper Menu.

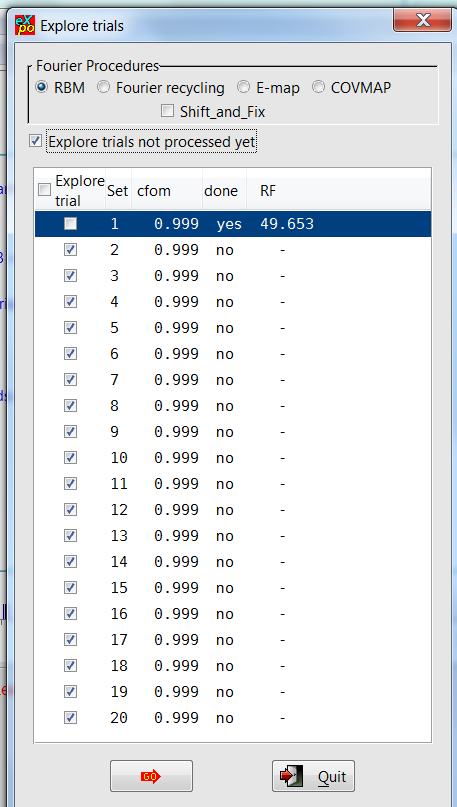


The following window is opened



and the CFOM values, for each saved trial, can be read. The highest CFOM value could not correspond to the correct solution while subsequent different trials may be successful (in the standard run by Direct Methods only the highest CFOM figure of merit phasing trial is automatically processed).

Check the button in the first column to decide which trial will be developed and press the button http://www.ba.ic.cnr.it/softwareic/expo/wp-content/uploads/sites/2/2016/12/NewItem52.png. If you check the button **Explore trials not processed yet**, all the trials not already explored will be automatically selected and developed.



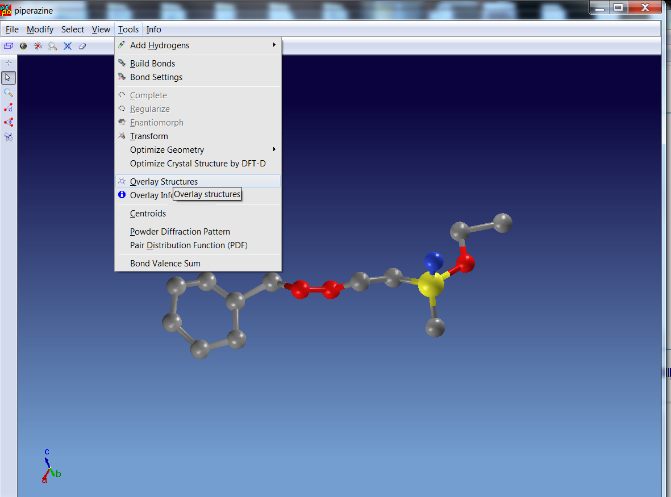
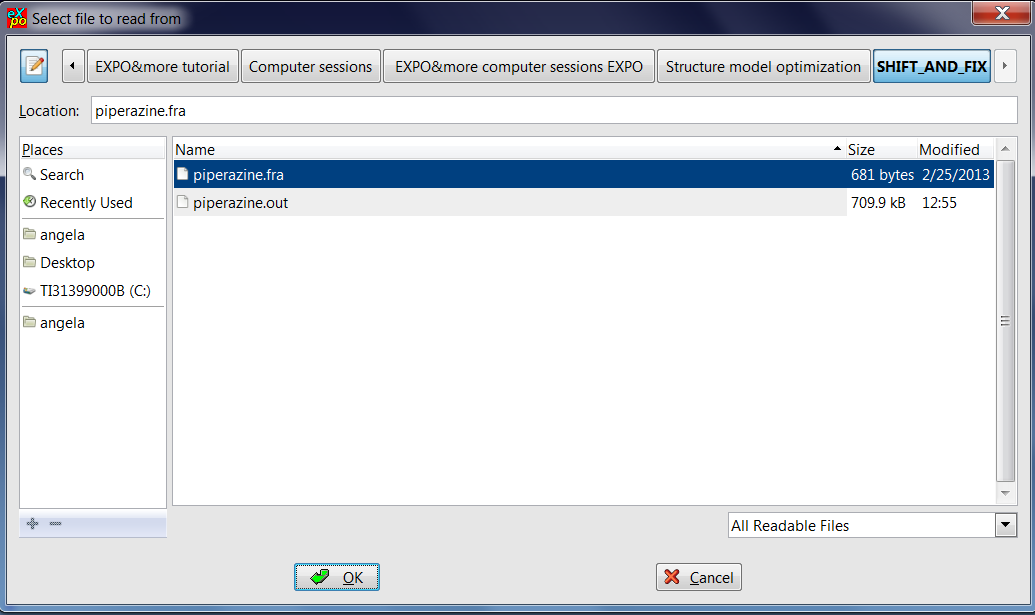
Click on **GO**.

The model first ranked by RF corresponds to the correct solution (the chemical label should be corrected: click on the Selection Mode icon  from the vertical menu of the JAV molecular viewer, left-click on the wrongly labelled atom position, right-click > Change Species and select the new label).

**Comparison with an external model**

The obtained solution can be compared with the published fractional coordinates contained in the piperazine.fra file (or LaTi\_true.cif if the example of default correct solution is using). It can be done by the following graphic pathway:

**Tools > Overlay structures** in the upper Menu of the JAV molecular viewer and select piperazine.fra (or LaTi\_true.cif if the example of default correct solution is using) and **OK**

The two models are superimposed and information on comparison can be output:

**Tools > Overlay Info** in the upper Menu of the JAV molecular viewer

