

MVP-Fit User Guide

1. Flexible fitting of one atomic model into one EM density map

1.1 Load EM density map

Click File->Open, choose format (*.map;*.mrc) to open EM data in CCP4 format with postfix .map or .mrc.

Click Edit->EMMesh/EMpoints/EMSurf/ to change visualization styles of EM density map. It's better to use mesh or isosurface when doing fitting. Click Edit->NoEM to hide the visualization of EM data.

1.2 Load atomic model

Click File->Open, choose format (*.pdb;*.ent) to open atomic structure in pdb format with postfix .pdb or .ent. After the EM file and pdb file are loaded, the EM isosurface will be semitransparent.

Click View->Backbone/Spacefill/Wireframe/Sticks/Ballstick/Bspline/Ribbons/Strands/Cartoon to change the style of atomic model. It's better to use the reduced representation Backbone when doing fitting. During the flexible fitting, it is better not to use modes Bspline/Ribbons/Strands/Cartoon since the recalculation of the smooth curve requires more time.

Click Color->Pure/Chain/CPK/Structure/Amino/Sharply/Group/Hydrophathy/Polarity/Acidity/Charge/Depth/Movable to change the color mode of atomic model.

1.3 Load parameter file

If there is a text file named para.txt in the same directory as that of the atomic model, this file will be loaded. Totally there are six lines in the file and each line contains one float number, which stand for the translation value in X, Y and Z axes, rotation angle in X, Y and Z axes. If there is no this file, the program will start from zero.

1.4 Load movable region file

If there is a text file named flexible.txt in the same directory as that of the atomic model, this file will be loaded. The first line in the file is an integer N which is the number of flexible loop regions. There are other following N lines, each of which contains two integer numbers which are the starting and ending residue numbers of each flexible region. If there is no this file, the program only can do rigid-body movements to this atomic model.

Click Color->Movable to see the flexible region in white while the color of the other region keeps the same as that of Group mode.

1.5 Change the threshold of EM density

Type Z/X to decrease/increase the threshold value. The mesh or isosurface will be reconstructed. This helps choose the best density threshold to accommodate atomic models in the isosurface.

Type J to see the value of current density threshold.

1.6 Rigid-body movements to the atomic model

Type A/S to translate the model in X direction forward and backward.

Type D/F to translate the model in Y direction forward and backward.

Type G/H to translate the model in Z direction forward and backward.

Type Q/W to rotate the model along X axis forward and backward.

Type E/R to rotate the model along Y axis forward and backward.

Type T/Y to rotate the model along Z axis forward and backward.

Type J to see the values of current three translation values and three rotation angles.

1.7 Translate one region

Type C until movetype=1. Type B/N to select the ending residue of the region. Type M/, to select the starting residue of the region. The ending residue can be any of the flexible residues or the end of the model. The starting residue can be any of the flexible residues or the starting of the model.

Type V to select the moving direction. 0/1 means along X axis forward or backward. 2/3 means along Y axis forward or backward. 4/5 means along Z axis forward or backward. The three axes are shown in conjunction with the starting and ending residues. This helps to avoid moving in the wrong directions.

Type ; to make the translation after setting the flexible region and direction. Keep clicking will keep doing the same operation until there is no hope to satisfy all the clash, bond length and bond angle restraints.

Type J to see the range and direction of the region under translation.

1.8 Rotate one region

Type C until movetype=2 or movetype=3. movetype=2 means rotating with the starting residue in the flexible region as the pivot while movetype=3 choose the ending residue as the pivot.

Type V to select the rotation axes. 0/1 means along NC α axis forward/backward while 2/3 along C α C axis. The rotation axis is shown in conjunction with the pivot residue. This helps to avoid rotating in the wrong directions.

Type ; to make the rotation after setting the flexible region and direction. Keep clicking will keep doing the same operation until there is no hope to satisfy all the clash, bond length and bond angle restraints.

Type J to see the range and direction of the region under rotation.

1.9 Save the modified atomic structure

Click File->SavePDB to save the transformed atomic model to .pdb file.

Click File->Save Para to save the three translation values and three rotation angles to a text file.

2. Rigid-body fitting of multiple atomic models into one EM density map

2.1 Load EM data and all the models simultaneously

Click File->Open EM+PDB to open the EM density map in CCP4 format and all the model files.

There should be one text file named modelnames.txt in the same directory as that of the EM data.

The first line in the file is the total number of models M . The following M lines are the names of the models which also should be in the same directory. The maximum number of models is set to 40.

2.2 Load parameter file

If there is a text file named para.txt in the same directory as that of the EM density map, this file will be loaded. Totally there are $6*M-1$ lines in the file if you want to preset the translation values

and rotation angles for the top M_I models. The parameters of the remaining models are set to zero.

2.3 Choose the movable model

Type K/L to change the model which needs to transform.

Type J to see which model has been selected.

2.4 Rigid-body movements to the selected model

Type A/S to translate the model in X direction forward and backward.

Type D/F to translate the model in Y direction forward and backward.

Type G/H to translate the model in Z direction forward and backward.

Type Q/W to rotate the model along X axis forward and backward.

Type E/R to rotate the model along Y axis forward and backward.

Type T/Y to rotate the model along Z axis forward and backward.

Type J to see the values of current three translation values and three rotation angles of the selected model.

2.5 Save the current transformed atomic structure

Click File->SavePDB to save the transformed atomic model to .pdb file of the current movable model.

Click File->Save Para to save the translation values and rotation angles of all the models to a text file.

3. Other supporting functions

Click Export->Image to save the screen as .png image file.

Click Option->Specular to increase the environmental light.

Click Option->Background to change background color.

Click Option->Full Screen to view the procedure in the full screen. Type Alt+S to switch to normal mode. Type Esc to exit the software.

Click Option->Lable to view the atomic model with residue label.

Click Option->Chessboard to view the chessboard plane.

Click Option->Axis to view the three perpendicular axes.

Click Option->FPS to get the number of frames per second.

Click Option->Movie to view the dynamic procedure.