PROCEDURE

3dRPC installation

1| To download 3dRPC package, visit the 3dRPC webpage (http://biophy.hust.edu.cn/downloads/3dRPC.tar.gz).

2| Set running environment for 3dRPC. Add the following lines to your '~/.bashrc':

```
export HOME_3dRPC=/home/XXX/3dRPC/
export X3DNA=${HOME_3dRPC}/ext/X3DNA/
export PATH=$PATH:${HOME_3dRPC}/ext/fasta/
```

Type the command in your terminal:

```
source ~/.bashrc
```

3| Download and install libraries. Three external libraries are required by 3dRPC: FFTW(http://www.fftw.org/download.html), BLAS(http://www.netlib.org/blas/) and LAPACK(http://www.netlib.org/lapack/). The default path of libraries is '${HOME_3dRPC}/lib/'.

4| Make FASTA programs and DSSP programs. The source code of FASTA is located on '${HOME_3dRPC}/ext/fasta/' and DSSP is located on '${HOME_3dRPC}/ext/dssp/'.

5| Make 3dRPC program from source code. The command is given below:

```
cd ${HOME_3dRPC}/source
make
```

Docking by RPDOCK

6| Prepare two pdb structures for docking, with one being protein and the other one being RNA. For example, 1DFU_r_u.pdb and 1DFU_l_u.pdb.

7| Prepare the parameter file for RPDOCK. The parameter file must follow the following format:

```
RPDock.receptor = 1DFU_r_u.pdb
RPDock.receptor.chain = V
RPDock.ligand = 1DFU_l_u.pdb
RPDock.ligand.chain = CB
RPDock.outfile = 1DFU.out
RPDock.grid_step = 1
RPDock.out_pdb = 10
```

The parameter file is explained in TABLE 1.

TABLE 1 | Explanation of parameter file for RPDOCK 'RPDOCK.par'

RPDock.receptor = 1DFU_r_u.pdb	file name of protein structure
RPDock.receptor.chain = V	chain id of protein
RPDock.ligand = 1DFU_l_u.pdb	file name of RNA structure
RPDock.ligand.chain = CB	chain id of RNA
RPDock.outfile = 1DFU.out	output file name of RPDOCK

RPDock.grid_step = 1	grid step of RPDOCK, 1 is recommended
RPDock.out_pdb = 10	number of complexes generated

8| Run RPDOCK by the following the command line:

$HOME_3dRPC/source/3dRPC -mode 9 -system 9 -par RPDOCK.par

RPDOCK.par is the parameter file described previously. After docking is finished, RPDOCK will gererate an output file '1DFU.out' and number of docked complexes ('complex1.pdb' … 'complex*.pdb'). An example of output file is shown below:

```
G_DATA  13  0   -946.00  13  25  1   3   48.0 0.0  0.0
G_DATA  10  0   -897.00  10  25  5   2   36.0 0.0  0.0
G_DATA  14  0   -858.00  14  25  2   3   48.0 0.0  0.0
```

Each line represents a docked complex with related information contained(TABLE 2). RPDOCK is a rigid-body docking procedure and the docked complexes depend on the translation vector and the rotation angles.

TABLE 2 | Explanation of information contained in the output file of RPDOCK.

Column 4	RPDOCK score
Column 6~Column 8	translation vector
Column 9~Column 11	rotation angles

9| Generate complexes by the following command line:

$HOME_3dRPC/source/3dRPC -mode 9 -system 8 -par RPDOCK.par

RPDOCK.par is the same parameter file that is used for docking. Users can change the number of complexes generated.

scoring on RPDOCK decoy

10| Prepare the parameter file for scoring. An example of the parameter file is shown below:

```
RPDock.receptor = 1DFU_r_u.pdb
RPDock.receptor.chain = V
RPDock.ligand = 1DFU_l_u.pdb
RPDock.ligand.chain = CB
RPDock.outfile = 1DFU.out
predicting.input_potential = ../../dat/RPDock.potential
predicting.score_output = complex.score
predicting.Resi_Resi_Inter_Predict_Cutoff_Min = 0
predicting.Resi_Resi_Inter_Predict_Cutoff_Max = 15
predicting.protein_protein_interface_cutoff = 20
```

TABLE 3 Explanation of the parameter file 'scoring.par'

RPDock.receptor = 1DFU_r_u.pdb	file name of protein structure
RPDock.receptor.chain = V	chain id of protein
RPDock.ligand = 1DFU_l_u.pdb	file name of RNA structure
RPDock.ligand.chain = CB	chain id of RNA
RPDock.outfile = 1DFU.out	output file of RPDOCK
predicting.input_potential = ../../dat/RPDock.potential	fixed parameter
predicting.score_output = complex.score	output of scoring

predicting.Resi_Resi_Inter_Predict_Cutoff_Min = 0	fixed parameter
predicting.Resi_Resi_Inter_Predict_Cutoff_Max = 15	fixed parameter
predicting.protein_protein_interface_cutoff = 20	fixed parameter

11| Run DECK_RP by command:

${HOME_3dRPC}/source/3dRPC -mode 2 -system 3 -par scoring.par

An output file 'complex.score' is generated. Its format resembles the output file of RPDOCK (step 8) except that the column 4 is the value of DECK_RP energy.

scoring on independent complexes

12| Prepare a list of complex structures to be evaluated by following the format:

complex1.pdb V CB

complex2.pdb V CB

The first column is the file name of the complex structure, the second column is the chain id of protein and the last column is the chain id of RNA.

13| Prepare the parameter file for scoring by the following format:

predicting.pdb_list = complex.list

predicting.score_output = complex.score

predicting.input_potential = ../../dat/RPDock.potential

predicting.Resi_Resi_Inter_Predict_Cutoff_Min = 0

predicting.Resi_Resi_Inter_Predict_Cutoff_Max = 15

predicting.protein_protein_interface_cutoff = 20

TABLE 4 Explanation of the parameter file 'scoring.par'

predicting.pdb_list = complex.list	list of complexes
predicting.score_output = complex.score	output of scoring
predicting.input_potential = ../../dat/RPDock.potential	fixed parameter
predicting.Resi_Resi_Inter_Predict_Cutoff_Min = 0	fixed parameter
predicting.Resi_Resi_Inter_Predict_Cutoff_Max = 15	fixed parameter
predicting.protein_protein_interface_cutoff = 20	fixed parameter

14| Run the command to score the complexes in the list:

${HOME_3dRPC}/source/3dRPC -mode 2 -system 0 -par scoring.par

According to the parameter, the output of scoring is saved in the file 'complex.score'. An example of output is shown below:

complex1.pdb -48.9526

complex2.pdb -30.4867

The first column is the name of the complex and the second column is the corresponding energy given by DECK_RP.