RSRef2000 Documentation Index

Installation

Running RSRef2000

There are 3 separate ways that RSRef can be run:

Command-line execution

For batch-mode refinements, perhaps of an entire macromolecule.

Parameter file format
Explanation and example of the parameter file used explicitly in command-line execution, and implicitly in the other forms of execution.
See also GUI Editor for full documentation of the parameters.

Using the Graphics-user-interface (GUI)

(This documentation contains the fullest description of the refinement parameters.)

Using the Interface with the modeling program O (with or without the GUI)

Accessory programs

SelectCoord and ReExpand:

Programs called by the refinement routines for the selection of coordinates, symmetry expansion, weighting & format changes.

Installation of RSRef2000

Introduction

Installation instructions for local real-space refinement package, RSRef2000. Written by Chapman, Korostelev, and Bertram (2000). This is a module for CNS, version 1.0.

How to install

All necessary executables will be created in the following 4 steps on a Unix platform:

1. Uncompress the .tar file:
   tar xvf RSRef2000.tar
2. In the newly formed directory find Makefile and edit it. You will need to enter the absolute paths of several directories, as well as some machine-specific compilation flags. Just follow the INSTALLATION steps in the makefile.
3. Run the Makefile (type "make").
4. In your .cshrc file add an environmental variable, RSdir, pointing to the current directory. For example, "setenv RSdir /ser/c/users/RSRef2000".
5. In your .cshrc file add “set path=(.)”.

If you use a “FRONT END” machine, then go to the "/front_end" subdirectory and read the README file. (A “FRONT END” machine is one where you will be running the molecular graphics package O, if different from the present machine that is called “REMOTE”. Either ***Unix*** or ***Windows*** workstations may be used as a “FRONT END” machines.)

Attention: Python should be installed prior to using RSRef2000 scripts. It may be downloaded from www.python.org for most platforms.

Troubleshooting

(1) At the compilation or linking stage error messages appear and the executable cns_LOC.exe is not created:

There may be a problem with installation of CNS on the machine you are using. For example, the absence of some libraries (complib, etc.) leads to an error. To figure out if this is a problem one should try installing CNS without RSRef2000 - when successful install RSRef2000.

Command-line execution of RSRef2000

rsref.py - RSRef2000 command-line execution

Syntax:

rsref.py *parameter_file* [-r] [-nostat]

-r if the refinement is to be run on a remote computer

-nostat cancels the default window of refinement statistics

Description

rsref.py is a Python script that runs the programs (Selectcoord, Refinement by CNS, Reexpand) in a batch of real-space refinement. It controls the various programs coordinately using parameters read from *parameter_file* which specifies, for example, whether optimization is by conjugate gradient or simulated annealing, the residues to be refined *etc*..

Simulated annealing refinement should be used if large changes are required (to get out of a local minimum). Conjugate gradient is appropriate for conservative refinement near the optimum.

Environmental Variables

All computers (both local and remote):

RSdir – the full path of directory which contains the RSRef2000 installation, *e.g.* ser/c/users/RSRef2000. This directory should already contain subdirectories pscripts, omacros etc. if correctly installed.

Unix operating systems:

RSdir would normally be set automatically on log-in with a command such as setenv RSdir ser/c/users/RSRef2000 in .cshrc for c-shell users.

Windows operating systems (front-end workstation):

RSdir is set in Start ▸ Control Panel ▸ System ▸ Environment.

Additional requirements for the Unix computer running RSRef2000 locally or as a remote compute-service:

Environmental variables for CNS. Normally, this is done on log-in with a command such as source /full_path_for_CNS/cns_solve_env in .cshrc for c-shell users. See the CNS for full details.

Additional requirements for an optional front-end unix or windows workstation running RSRef2000 on a remote computer:

REM_MACHINE – the account and computer name where RSRef2000 is to be run remotely, in the format account@computer.

REM_DIR - the full directory path containing the RSRef2000 installation on the remote computer.

These would normally be set on log-in the same way as *RSdir* (see above) under both unix and windows. So, the following example commands in .cshrc would be appropriate for c-shell users: setenv REM_MACHINE user@leu.am.msu.edu; setenv REM_DIR leu/users/RSRef2000.

Temporary scratch files

These are created in the RSRef_Temporary_Fls subdirectory of user's account on the remote and local computer where refinement is run. The files are purged following normal completion of the refinement.

RSRef2000 GUI Editor

Introduction

The RSRef2000 Editor provides a graphical user interface (GUI) for controlling refinement jobs. Control parameters (settings) are entered into a form which may be

saved to a file (*.prm) or used to run a refinement job directly from the GUI. When refining from within O, the GUI should be left running throughout the modeling session.

Preparation for Use:

The GUI is written in Python using Tkinter, a standard object-oriented interface to the Tk.

Unix users: the Tk library should be installed (it may not come with the Python). The LD_LIBRARY_PATH environmental variable should point to the Tk installation directory, using, for example the following command in the .cshrc file:

```
setenv  LD_LIBRARY_PATH /usr/local/lib
```

Under Windows, Python (www.python.org) already contains the Tk library.

Syntax:

rsrefGUI.py *parameter_file* - for making corrections to an existing parameter file. Specifying the parameter_file is optional – a new parameter file may be created or an existing parameter file may be uploaded.

Explanation of items:

Starting coordinates

PDB format file name. If refinement is carried out from "O" this field is not used – specify as "none".

Output coordinates

Filename. If refinement is carried out from "O" this field is not used – specify as "none".

Map file

Full path of electron density map in DSN6, or OMAP, format. The map should be to the remote machine if one is used as a compute-server.

Symmetry file

Contains non-crystallographic, *and crystallographic*, symmetry operators to be applied to the initial coordinates. It need contain only those operators that bring coordinates into the refinement region or the neighboring margin. The program does not otherwise know about space group or unit cell translations, so the subset of operators that generates neighbors should be entered explicitly. The program does not attempt to iteratively concatonate symmetry operators and/or cell translations - they must all be entered explicitly. The format is given in the selectcoord documentation. Selectcoord can also be used to determine which operators generate neighboring atoms as it can be asked to find atoms that fall within a particular distance of the first protomer, and will report the number found for each operator.

Summary log file

File name.

Low resolution limit and High resolution limit

Resolution limits that were used for creating electron density map.

Atom size cut-off

In calculating model density, contributions from an atom will be ignored if the atom center is farther than this distance. The default of 3.4 A is appropriate for a 3.0 A map. Up to a point, the larger the value the more accurate, but slower will be the calculation. The optimal should be dependent on the resolution but is larger than some expect, because it is important to include the ripples of positive and negative density that surround a map of an atom that has been resolution-truncated..

Refinement radius

Map pixels will only be used for the refinement if they fall within this distance of any refining atom. The best value is a compromise. The value should be small enough to favor the stronger and more reliable densities near atom centers, but large enough to include a statistically significant number of grid points. The default of 1.6 is appropriate for a 3. A map on a 1 A grid. "Refinement radius" should be decreased for accurate structures at high resolution, and increased for low resolution, or coarse grids, or to increase the convergence radius. Note that the Atom size cut-off should always be larger than refinement radius.

Region

Menu selection: **zone** or **sphere**. With "zone" one should supply residue numbers (First residue and Last residue) of a zone that will be refined. If "sphere" is chosen Radius and Center x, y, z coordinates of it should be supplied. *If crystallographic or non-crystallographic symmetry is present* (see **Symmetry file** option), the symmetry relationships between the refined region of the protomer and its copies will be retained. Selectcoord makes the symmetry expansion, creating the symmetry equivalent copies of the protomer, and reexpand restores symmetry between atoms that have been shifted independently.

Note that when refining a sphere the following applies: If atoms of the symmetry related subunit and not the 1st protomer are chosen to be refined, the coordinates of the 1st protomer will be changed in order to retain the symmetry. If more than one equivalent of an atom is chosen to be refined at once the symmetry relationship between them will be retained as well.

Margin

Residues within this distance outside a refinement region, zone or sphere, will not be refined (they will be fixed), but they will contribute to the calculation of electron density and to the stereochemical energy. If residues from a symmetry

related subunit fall in the margin, they will also be fixed while contributing to the overall refinement.

Refinement

Menu options controlling the type of optimization: conjugate gradient, slow cooling or quenching (fast cooling).

ED Weight

Weight on electron density term. There is no good way to predict a sensible value, as it depends on the absolute values of electron density values (and hence on absolute scaling of Fs) and also on the number of grid points per atom. So, trial and error is the norm. An approximate value can be obtained by matching the magnitude of the density residual to the stereochemical one. A better approximation would come by matching the sizes of the atomic derivatives for density and stereochemistry. However, ultimately the proof is in the pudding. The value should be adjusted until the balance between map-fit and stereochemistry is good, and cross-validated indices are optimized.

MD type

Menu for choosing between torsion angle dynamics and Cartesian dynamics. This is applicable for either slow cooling or quenching protocols. The recommended protocol is torsion angle dynamics. If this fails Cartesian dynamics should be used.

Starting temperature

Higher temperature limit of molecular dynamics. This is applicable for either slowcooling or quenching protocols. 2000 K is recommended for regions that are in reasonable shape. Values as high as 30000 K may be necessary to fix intransigent regions.

Drop temperature

Rate of slowcooling. (Recommended – 500 K if starting temperature is in range of 2000 K). Note that this parameter is ignored in quenching.

Buttons

Read

Read an existing parameter file. A name with full path should be given in the adjacent prompt.

A new window will be opened. Reading a new parameter file spawns a new GUI window (unfortunately in the Windows version, the original GUI window becomes hung).

Prepare for 'O'

Prepares macros and initializes the O - RSRef2000 interface. Needs to be used only once in each directory where O is to be run. See the documentation to the O - RSRef2000 interface before using this option.

Run from 'O'

Under Windows, after selecting the region to refine, the user will be prompted in O to push this button. Available only in Windows. (Under unix, the refinement runs automatically after selection of refining residues).

Save as

To save the parameters in the named file.

Run

To run a stand-alone refinement job with the current settings from the RSRef2000 GUI editor. Options (-r, for use of remote machine; -nostat, to cancel statistics windows) may be specified in the options field.

Quit

Exit the editor without saving the parameter file.

Parameter File Format

Introduction

The parameter file is a text file that may be created automatically by the RSRef2000 GUI editor or manually in a text editor. It contains information that will be used by rsref.py (see Running RSRef2000) for real-space refinement of local regions of macromolecules. Explanation for each entry is given in documentation for the RSRef2000 GUI editor.

An example of a parameter file is in the *sample* directory. It is largely self-documenting (see example), but the following may help the uninitiated. More detailed comments are in the standalone rsref module (RSRef2.0) documentation. Note that most of the options of the standalone rsref module are not implemented in RSRef2000.

Remarks

1. If a "remote" machine (compute-server - see Running RSRef2000) is used for refinement:

- Run_script should be set to '-r'
- The remote machine should have the Map file and NCS (non-crystallographic symmetry operator) file and the full paths should be specified in corresponding fields

    I. The rest of the files should be on the local "front end" machine. Full path should be specified if they are not in the directory from which rsref.py is called.
    II. Output files will be written to the "front end" machine.

2. A Region containing several residues starting from First_res and ending at Last_res is called a Zone.

Example

Note: parameters are fully documented in the page for the RSRef2000 GUI editor.

```
*RSRef parameter file.
*Set any parameter you do not use to "none".
Parameter_file = ak.prm
Run_script = -r

>>>>============================== Resolution range
Low_res_limit = 6.0
High_res_limit = 1.2

>>>>========================== Files used in real-space refinement
Starting_coord = ak.pdb
Output_coord= ak_refined.pdb
Map_file= Maps/anneal1.2final2.dsn6
Log_file= ak.log

>>>>============================== Crystallographic data
symmetry_file= none                    =(replace "none" with the name of the symmetry-operator file)
Atomsize = 3.4
Refsize = 1.6

>>>>============================== "Local Refinement" information

Region =  zone                 =(region to be refined. Choice: zone, sphere)
>> First_res and Last_res must be specified if a zone is to be refined
First_res = 2
Last_res = 3
Margin = 1.5                   =(of unrefined atoms that contribute to the calculated energy.)

>>>>============================== Minimization information
w_a=40.0                       =(weight for Electron Density component)
ref_scheme=slowcool            =(choice: conjugate, slowcool, constant)

>>>>=============== Molecular dynamics data
md_type = torsion              =(molecular dynamics type. Choice: cartesian, torsion)
start_temp=1700.0              =(for slow-cooling, or constant-temperature)
cool_rate=500.0                =(drop temperature; recommended cool_rate=500)

>>>>============================== end of parameter file.
```

Running RSRef2000 interactively from "O"

Setup

Following program installation, RSRef2000 needs to be set up in each directory in which O is to be run.

Warnings:

- The setup procedure creates a new User Menu in O. If the user menu has already been customized, its contents should be saved, and following setup, read into the file $RSdir/omacros/rsrefmenu.o. In this way both the options required by RSRef2000, and the user's will be displayed.
- Setup initializes a number of files. Edited / customized values may be lost if setup is run again in the same directory.

1. Run @RSdir/omacros/rsrefSetup.macro as a macro from within O. (*This option is not available under Windows*.) *RSdir* is the environmental variable that defines the full path to the RSRef2000 installation. Such environmental variables may not be accessible within the O program, so you will likely have to type the full path explicitly within O. Example:
   @/ser/c/users/RSRef2000/omacros/rsrefSetup.macro
2. Copy *$RSdir*/pscripts/rsrefGUI.py to the directory in which O is to be run. Run rsrefGUI.py and in the resulting session of RSRef GUI editor click "Prepare for 'O'" (this should only be done once per directory, even if repeating the setup). Then type @rsrefSetup.macro in the O window.

Input requested during initialization:

- Name of the molecule you want to refine ("mol" name in O)
- Name of the RSRef2000 parameter file with its absolute path. Note that this parameter file is changed and overwritten during refinement, so should be backed-up periodically to a file of a different name.

Running RSRef2000 from within O.

Under Windows, it is compulsory to be running rsrefGUI.py (that controls the graphics user interface), and it should be started once per O-session. *Under Unix*, it is recommended, but not necessary.

Aside from the selection of residues, this is the last time that refinement parameters may be changed under Unix. They may be edited with the graphics user interface (Windows or Unix) or through text-editing of the parameter file (Unix only). Note that saved parameters may be read from a file. Note also that the latest parameters will continue to be used until changed again, but need to be saved explicitly for use in another session.

If the setup has completed correctly, the O window should contain an RSRef menu with 4 options that (optionally) add residue selections to the parameter file:

RSRef

to pick the first and the last residues of a zone of residues to be refined.

Note that for both zone of residues and spherical region (below) the following applies: *If crystallographic or non-crystallographic symmetry is present*, the symmetry relationships between the refined region of the protomer and its copies will be retained. Only atoms of the selected region will be refined, while the atoms that fall within margin (determined in the parameter file) will be fixed during refinement. If atoms of the symmetry related subunit and not the 1st protomer are chosen to be refined, the coordinates of the 1st protomer will be changed in order to retain the symmetry. If more than one equivalent of an atom is chosen to be refined at once (for example, when spherical region is defined) the symmetry relationship between them will be retained as well.

RSRefSph

to pick an atom at the center of a sphere to be refined. The radius and the width of a margin containing non-refining atoms contributing to the energy calculation are entered from the keyboard.

RSRefxyz

Like RSRefSph, except that the coordinates of the center are entered by keyboard, not by atom-picking.

Del_RSRef

removes the object RSRef (when rejecting the changes made by refinement).

Under Unix, the macro will start refinement directly.

Under Windows, refinement must be started explicitly within the graphics user interface by clicking "Run from 'O'".

“Refinement completed, accept new coordinates Yes/No?”

Under both Unix and Windows, a refined partial model will be placed in an O object, RSRef, and can be inspected.

Answer yes or no to the question: “Refinement completed, accept new coordinates Yes/No?”. If yes, the refined region gets incorporated into the initial model. If no, the RSRef object can be cleaned up with Del_RSRef in the Rsref-O menu.

Files:

There are three input files for CNS. They may be changed if, for example, user-defined topology files are to be used:

$RSdir/pscripts/generateLOC.inp - input CNS file used for creating .mtf file before actual refinement.

$RSdir/pscripts/realcgLOC.inp – input CNS file used for conjugate gradient refinement.

$RSdir/pscripts/rsrefLOC.inp - input CNS file for simulated annealing refinement.

If both REMOTE and FRONT END machines are used, these files are located on the FRONT END machine. *Under Windows*, the files are being temporarily copied to the RSRef_Temporary_Fls directory on the REMOTE host where calculations proceed.

SelectCoord and ReExpand

Description

During the refinement process, all atomic coordinates are independently shifted, even when either crystallographic or non-crystallographic symmetry is present. Constraints between shifts must be applied in order to retain the symmetry relationships between the copies of the protomer. Selectcoord makes the symmetry expansion, creating

the symmetry equivalent copies of the protomer, and reexpand restores symmetry between atoms that have been shifted independently.

These programs run as part of refinement of macromolecules. Selectcoord also allows selecting the refining region of a macromolecule (zone or sphere - details in RSRef2000 GUI editor), atoms within the margin (RSRef2000 GUI editor) which will be fixed during refinement, and residues from neighbouring symmetry related subunits which are close to the refining region and also will be fixed. Fixed atoms are contributing to the overall energy *via* interaction with the refining atoms.

Note that when Selectcoord and Reexpand run as part of the distributed refinement routines, only a subset of the functionality and parameters are available.

Function

selectcoord - selects subset of coordinates, sets-up book-keeping for symmetry equivalents.

reexpand - reimpose (non-crystallographic) symmetry equivalence.

Syntax

selectcoord *(no command-line input/options)*. *May be run from the cshell script* as shown in the examples selectcoord_zone.* which may be found under subdirectory *pscripts*.

reexpand *init-file protomer-file expanded-file*

SelectCoord

The input is key-word directed. Comments, multi-line and redirected input are supported. Nested redirected input is given using @{file}, multiple line input using the "\" continuation character at the end of a line, and comments begin with "!". In the documentation, optional input is enclosed between [...], user-variable input should replace text enclosed within {...}. Input is free-format, but spaces are not allowed in strings.

Options specify coordinate files, symmetry operations to be applied and define a volume in which transformed coordinates must fall to be accepted. All the selection criteria must

be satisfied for acceptance, but not all criteria need be invoked. Atoms are accepted from any symmetry-equivalent of any residues for which at least one atom is in the defined region, but atoms within a residue can be output with different weights and designations for refining, fixing etc.

Files

[Input [=] {string}] [Output [=] {string}]

Coordinate files: no defaults are provided

Files Input = input.pdb Output = expanded.pdb

Symmetry_operator

[Name [=] {string}] [Rotation [=] ({real})]

[Translation [=] ({real})]

This is repeated for each operator.

Name: a suffix appended to the chain name to designate the symmetry equivalent. The default is blank for the 1st operator, "A" for the 2nd, "B" for the 3rd etc. The name should not exceed 2 characters if chain identifiers are present in the coordinates, 4 characters if not.

Rotation: the nine elements of a 3 x 3 matrix in the order conventionally written: 3 elements of 1st row, then 2nd row, then 3rd row. The default is a unit matrix. The symmetry operators are acting on column vectors, in an orthonormal basis.

Translation: three elements of a translational matrix, applied after the rotation in the forward transformation, i.e.

```
Symmetry_operator Name = B Rotation =
                         -0.50000 -0.80899 -0.30909 \
                         0.80899 -0.30893 -0.50009 \
                         0.30909 -0.50009  0.80893 \
            Translation = 0.00000  0.00000  0.00000
```

Sphere

[Center [=] ({real})] [Radius [=] {real}] [Margin[=] {real}]

Center: the position of the sphere; default = (0.0,0.0,0.0).

Radius: the radius of the sphere; default is enormous.

Margin: add (fixed or low weight) residues with any atom within Margin Å of the volume border. Atoms in the Margin are fixed, but they are used in energy calculations. If Margin is greater than zero, the margin is outside the volume, else inside.

Sphere Center = -10.5 15.2 3.5 Radius = 20.0

Box

[X_limits [=] {real}] [Y_limits [=] {real}]

[Z_limits [=] {real}] [Margin[=] {real}]

-- The lower and upper limits for the box; defaults to an all-inclusive box.

Margin: add (fixed or low weight) residues with any atom within Margin Å of the volume border. Atoms in the Margin are fixed, but they are used in energy calculations. If Margin is greater than zero, the margin is outside the volume, else inside.

Box X_limits = 0.0 100.0 Z_limits = 80.0 120.0

Neighbors

[Contact [=] {real}] [Accuracy [=] {real}] [Start_Zone = {text} End_Zone = {text}]

Contact is the equivalent of Margin, but for a zone. If Contact is greater than 0, accept only those symmetry-equivalent residues within Contact Å of an atom from selected atoms in the first symmetry equivalent (default = 5.0). **Accuracy** is the maximum acceptable error in rasterizing the coordinates when determining neighbors (default = 1.5).

The selection of residues comes either from **Sphere**, or **Box** commands, or from the following:

Start_Zone, End_Zone: specify a zone. Residues are specified as [chain|]residue. The wild-card character "*" is supported.

Neighbors Contact = 5.7 Accuracy = 1.2 \

Start_zone = A|5 End_zone = A|25

Plane

Origin [=] ({real}) 2nd_point [=] ({real}) 3rd_point [=] ({real})
[Margin = {real}]]

-- Only those atoms within the specified planes will be accepted. A plane is specified by three coplanar points and an optional translation along the normal.

Note that there are no defaults for the three position vectors, **origin, 2nd_point** and **3rd_point**. An error will occur if values are not supplied. The order of the points in the plane is important. If a 4th point is defined to be outside the plane, then the vectors (2nd_point - origin), (3rd_point - origin) and (4th_point - origin) should make a right-handed set. If **Margin** (default = 0.0) is positive, the plane is moved outward along the normal, if negative inward. **Plane** must be called for each plane required.

Plane Origin = 0.0,0.0,0.0 2nd_point = 0.52547,0.0,0.85081 \
3rd_point = 0.0,-0.35674,0.9342 Margin = 5.0

Reexpand

Background

There are 2 differents ways to select a “core” refining zone and to add symmetry equivalent neighbors:

- the primary structure, i.e. all atoms between residues x of chain a and y of chain b are to be refined.
- by location, i.e. all atoms within a sphere of radius r centered at point x are to be refined. The selection region can be a sphere, a rectangular box or more generally defined by a set of planes.

Around the core zone, a "neighbors" zone or Margin is defined, which contains all neighboring atoms within a threshold distance of any "core" atom, 5 Å for example. Atoms in the margin are not refined, but are used in energy calculations. A third "outer" zone is defined, containing all atoms in residues for which at least one atom is in the

Margin. These latter atoms are not refined, but their presence is required since stereochemical restraints cannot be applied on partial residues.

When reexpansion occurs after a refinement cycle, symmetry is enforced for all atoms that belong to these 3 zones. Shifts are computed in two steps: first the shift of the atom in the protomer is computed by:

$$\mathbf{d} = 1/(w_i) \; . \; \text{Sum}_{i=0}^{n\_s} \{ w_i \mathbf{R}_i^{-1} \mathbf{d}_i \}$$

where $\mathbf{d}_i$ is the independent shift of the ith symmetry equivalent, related to the protomer atom by the symmetry operation $\mathbf{R}_i$, i running through all symmetry equivalents of current atom presents in the 3 zones. Then the shift is applied to all copies. This former equation involves weights w_i, which are 1 for the atoms belonging to the core zone, 0 for the outer zone atoms. This scheme is valid for all atoms and allows atoms which do not belong to the protomer to be shifted.

Input/Output Files

Either PDB or TNT ATOMC formats may be used. The file types are determined from the ".pdb" or " .cor" extensions, respectively.

selectcoord creates an equivalence file (extention *.eqf), containing all information pertinent to symmetry reexpansion. The name of the file is built from the output coordinates.

selectcoord's chain identifiers have names that are a subset of TNT's, i.e. 4 characters maximum. If selectcoord is used in context of CNS or X-PLOR chain identifiers should contain 1 character. Symmetry operations generate new chains with names that are extensions to the original chain name, when this extension scheme is possible. For example, a viral capsid is made of 4 different chains (1-4), which are copied by 8 symmetry operators (A-H), including the identity matrix. Application of the "A" operator on chain "1" will generate output chain 1_A. In most cases, the chain name should not exceed one character, 2 characters for the symmetry operator name, 1 character being reserved as separator. This can cause problems when converting back to a PDB file, because only one chain character is allowed in this format.

Limitations

Current version of selectcoord is supposed to be used for not very large regions of macromolecules. The program may stop if number of selected residues exceeds 600-1000 residues.

Credits

Program written by Eric Blanc, as a near-re-write of expcoord (M.S. Chapman).

Other Files:

${RSdir}/selectcoord ${RSdir}/reexpand - executables.

${RSdir}/source/ [selectcoord.c reexpand.c eqFile.c expandCoord.c mask.c oSymm.c] source codes.

${RSdir}/source /Makefile – makefile for selectcoord and reexpand

${RSdir}/source/Lib/Libraries/ [libcrystal.a libtoken_io libcoords.a libmatrixvector.a] object libraries.

${RSdir}/source/Lib/ [Coordinates/* Crystal/* Matrixvector/* Token_io/*] directories with makefiles and sources of library routines.