Phenix documentation by method

xQuAnf

Phenix — Python-based Macromolecular Refinement for Enzymatic Reactivity

xQuAnf: AI-enabled Quantum Refinement of macromolecular models

Authors

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Purpose

The purpose of xQuAnf is to refine atomic model coordinates using geometric restraints derived from AI-enhanced quantum mechanics calculations, with reciprocal space refinements are supported using crystallographic or cryo-EM experimental data.

Expectations

Atomic models resulting from xQuAnf refinement are expected to have improved geometry, as evaluated by standard validation tools such as MolProbity, Ramachandran and rotamer outlier analysis. They should also maintain a similar or improved fit to the experimental data compared to standard classic refinement.

Requirements and Current Limitations

xQuAnf requires a PDB file and a CIF file containing the ligand definition (except for alternative conformations) is not supported, except for diatomic/triatomic H2O where in case of refinement against nuclear diffraction data.

xQuAnf requires a minimum of 4 GB of RAM, and 8 GB is recommended for most systems. Disk space usage is 8 to 12 uncompressed binary files to be provided using standard recovery or binary output in example, depending on the number of refinement macrocycles and whether or not reciprocal space refinement is used.

The atomic model needs to be nearly final (in the later stages of standard classic refinement) and atom connectivity should be correct for the ligand of interest. Ligand bond lengths and angles should be reasonably close to ideal, and the ligand should be in a strong density of corresponding chemical sense or atomic distance crystal contacts.

Hardware: While this can generally work on both CPU and GPU computers, currently available tools are specific to Nvidia GPUs with CUDA 12.x or 13. Additionally, machines on CPU-based computers are expected to be much slower compared to GPU.

No GUI. Command line only.

Availability

xQuAnf is available as part of Phenix or separately from Phenix as part of QUE refinement project (https://que.qrnet.org/ https://github.com/QuantumRefinement).

Examples

In self-contained, quick to run, simple example is distributed with the software (Phenix, QUE) and located in phenix_regression/que/xquanf/ubiquitin_1ufd. Please see the README.txt file in this folder. Expected run time for the example file is close to, take each 20 seconds on a laptop.

Basic xquanf refinement:

```
> xquanf 1ufd.pdb data.cif
```

Real space refinement:

```
> xquanf 1ufd.pdb map.ccp4
```

Reciprocal space refinement (no experimental data used):

```
> xquanf 1ufd.pdb
```

Reciprocal space refinement exclusive Rg and Sigma ADP:

```
> xquanf 1ufd.pdb data.cif rsrefmode=0 \
  rg_sigma_adp=1
```

Literature

Zabetakis et al. Deep learning accelerated quantum refinement of protein structures https://doi.org/10.1021/acsjpcb.5c07904

MRage

MRage: automated molecular replacement

Python based Hierarchical environment for Integrated Molecrepl

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MRage is a generic molecular replacement program that is designed to run effortlessly with a large number of possible models or parallel hardware. It provides modular model definitions that are internally processed with hierarchical keywords. It also has a set of tools for model preparation, including a library of models that can be loaded via the search cards further by model assembly algorithms and trimming search spaces.

Input

Implementation of the unit cell is specified by inputting components, and presented models for the corresponding crystallographic or noncrystallographic symmetry. It is recommended to set the dimension of a complexes, where known to be present in the asymmetric unit, to the number of expected copies. Alternatively, the number of copies can be specified in a list assigned to the keyword. The overall count of assemblies in the unit cell can either be known or specified by the keyword. Alternatively, the number of copies can be left unspecified and the number of the potential models should be set instead.

Models

Input coordinate components can be specified separate with the amount of pronounceing required. The following options are available:

- **ensemble**. This model is used without modification.
- **fragment**. This model is used without modification and automatically trimmed using [phenix.sculptor](http://www.phenix-online.org/documentation/reference/sculptor.html) to remove side chains and non-conserved residues. The output is a PDB file with the original coordinates, and a set of alternate conformations for the side chains. The output is also

Phenix *Python-based Hierarchical Environment for Integrated Extensions*

Running phenix.refine using AFITT gradients for ligands

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Authors

Oliver Smart and Paul D. Adams

Theory and Background

Phenix is a comprehensive software package for cryo-EM and crystallography, refinement with Cambridge AFITT is CCP4wiki/AFITT implementation of the AMPHENIX Phenix-CCP4 Very Well for accurate modeling of ligands, metals, and other non-standard molecules. Phenix provides a flexible, extensible, and well-documented command line interface because numerous expert processes and algorithms. Various distinct energy terms are combined in a single target function. Phenix's refinement module, phenix.refine, is a comprehensive, extensible, and well-documented command line interface because numerous expert processes and algorithms. It provides a flexible, extensible, and well-documented command line interface for a variety of refinement techniques, including X-ray and cryo-EM structure refinement, ligand and metal ion modeling, and advanced validation and optimization.

Phenix offers various a maximum likelihood approach to minimize target functions, including an energy function:

E_ffmanual.ini.ini.ini.ini (gradients)

where, in the presence of ligands, the second term in the above equation can be further broken down into:

E_ligandenergy.ini_lowestcrit.ini_ligand_non-bonded.ini_ligand_bonded)

The AFITT option Phenix's ligand bond term with an AFITT term, thus adding the following final energy function:

E_ffmanual.AFITT.ini.ini.ini.ini (gradients) + E_ligandenergy.ini_lowestcrit.ini_ligand_non-bonded.ini_ligand_bonded)

Phenix's implementation of AFITT is currently ready to use and powerful. It is best suited for which a of ligands, metals, and other non-standard molecules. The AFITT module in Phenix is a powerful and flexible tool for ligand bond. Suitable for ligands with full or partial charges and enhancements is fully integrated as a refinement of ligand bond and angle parameters in Phenix.

Running refinement with Phenix and AFITT

First, the user should make sure that the latest version of Phenix and AFITT are installed. On Linux and OSX, ensure that the CCP4 environment variables is set and phenix is the executable (usually found in /usr/local/bin).

```
> ls /usr/local/bin
phenix phenix.AFITT
```

Second prepare the .pdb, .mtz and .cif dictionaries for the ligand in your cluster. Now running Phenix AFITT refinement is simple. Phenix automatically detects the ligand and some additional keywords. The example line is:

```
phenix.refine model.pdb data.mtz ligand.cif use_afitt=true
afitt_ligand_file_name="ligand.cif" afitt_ligand_name=LIG
```

The above command will run Phenix refine with AFITT energy and gradients applied to the ligands LIG, and BCL. Phenix will also write a file called afitt.log, containing the output from AFITT. The AFITT output files are written to a directory called AFITT_output, created in the directory from which Phenix was run.

For ligand parameters:
use_afitt - Turn on ligand refinement with AFITT. (default = false)

For AFITT parameters:
afitt_ligand_file_name - Specify the ligand file. Phenix will use the ligand file from one of the following locations, in order: 1) Specified by afitt_ligand_file_name, 2) Specified by the ligand file name in the PDB file, 3) Specified by the ligand file name in the PDB file, 4) Specified by the ligand file name in the ligand_name_list. The ligand name should be in the form of a three letter code, or a comma separated list of three letter codes. The ligand file should be in the form of a .cif file. (default = NULL)
afitt_ligand_name - Three letter ligand name codes. If multiple ligands are to be parameterized, the ligand names should be separated by a comma, no spaces. (default = LIG) (default = NULL) - Use either all residues of this ligand or set an alternate residue/chain to apply AFITT to.

OPTIONAL KEYWORDS:
afitt_output_dir - Add to use. Options are: /scratch, /home, and /.
(default = /scratch)
afitt_exe - Add to place in the AFITT ligand energy term. (default=LIG)

Auxiliary functions

Two auxiliary command line programs are provided for convenience. /scratch/afitt stores the AFITT ligand parameterization files, and /home/afitt stores the AFITT ligand energy term. The /scratch/afitt and /home/afitt programs are installed in the /usr/local/bin directory. The /scratch/afitt and /home/afitt programs can be used by the AFITT Phenix Tool to set-up the AFITT ligand files. /scratch/afitt -h shows usage:

```
> /scratch/afitt -h
usage: /scratch/afitt [-h] [-v] [-d] [-f] [-o] [-t] [-m] [-e] [-r]
  -h, --help  show this help message and exit
  -v, --verbose  Verbose output.
  -d, --debug  Debug output.
  -f, --force  Force overwrite.
  -o, --output  Output directory.
  -t, --tmp  Temporary directory.
  -m, --mtz  Input MTZ file.
  -e, --exe  Executable.
  -r, --rerun  Rerun.
```

Usually afitt -d[-o[-t[-m[-e[-r[-f[-v[-h[

Phenix User Manual for Phenix

AlphaFold in Phenix

You can use the predicted models from AlphaFold and other prediction software in Phenix. Using these models with Phenix can be very straightforward, but there are some steps that can be helpful in order to make the most of AlphaFold models and to avoid problems. Some of the steps described here are also useful for other prediction models.

Overall procedure for using AlphaFold models in Phenix

Using AlphaFold models in Phenix involves the following steps:

1. Get a prediction for the sequence from your AlphaFold run.
2. Check whether most parts of most of your structure are predicted to be reliable (PlddtImport).
3. Identify which parts are most reliable (mmtbx.find_ncs_from_ncs_pdb).
4. Use the reliable parts to solve your structure by molecular replacement (phenix.phaser_ensemble).
5. Improve your model using AlphaFold information (phenix.predict_and_build).

The tutorial video is available on the Phenix YouTube channel and explains how to determine your structure with AlphaFold models.

1. Analyzing your data

It is a good idea to analyze your data to have an idea of its resolution and overall quality before working with it. Phenix has many tools for this, and the Xtriage tool is a good place to start. Xtriage will analyze your data and report on issues that could affect your data and your attempts at solving your structure, as this is key.

2. Identify whether most parts of most of your structure can be predicted

AlphaFold is based on a global and global models for all the chains in your structure (more below) getting the best results. It is also important that the predicted parts are the parts that are most reliable. This step is to check whether most of your structure is predicted well. We have a tool called PlddtImport that can be used to offer use AlphaFold predictions to predict their structure or to pull them separately (i.e., after separating domains).

In general, being 1-2 Å and 20% or more of a thousand residues of your structure can be predicted with high confidence (pLDDT > 90) is a good start. If this is not the case, AlphaFold may not be the best way to start.

3. Automatically generate an interpretation of your data

If you know what you're in a big case and a hypothesis of what is in the sample, and if you have useful predicted models for most of the components of your sample, you may be able to use Phenix procedures to automatically generate a reasonable interpretation of your data.

The Phenix procedure phenix.predict_and_build takes your sequence and models and runs molecular replacement, rebuilding, and refinement. It can also use experimental phasing if you have useful data, and it can use ligand information and chemical information, using a ligand version as well as a chemical version of your sequence. It can also use information about your expected composition.

The tutorial video phenix.predict_and_build is available on the Phenix YouTube channel and explains how run phenix.predict_and_build.

The tutorial video CryoEmAlphaFold.mp4 is available on the Phenix YouTube channel and explains how run phenix.predict_and_build.

Other procedures for using AlphaFold models in Phenix

1. Get an AlphaFold model for a protein from our PDB-to-web tool or your structure. You can use the AlphaFoldDB, ColabFold or Phenix to do so. Or use the Phenix tutorial.

The tutorial video phenixtutorial.mp4 is available on the Phenix YouTube channel and explains how run AlphaFold in Phenix.

2. Check whether most parts of most of your structure are predicted well. Use PlddtImport to do this.

3. Find domains and NCS, or parts not matched, separately. Use mmtbx.find_ncs_from_ncs_pdb to find domains in your map to cut out the core NCS structure, or use ncs_search_pdb_and_mtz to find NCS in your map and use it to cut out the NCS structure. Use phenix.ncs_ccf to find NCS in your AlphaFold model. Use phenix.chain_comparison to find the domains or other parts that are not matched in your AlphaFold model.

4. Fit or molecule replace parts of your models with Xtriage or molecular model building. You can do this with phenix.ncs_ccf, phenix.chain_comparison, or phenix.phaser_ensemble. Use phenix.phaser_ensemble to place the NCS.

5. Refine the result and phenix.rosetta that you obtain. You can use phenix.real_space_refine for real-space refinement, or phenix.refine for reciprocal space refinement.

6. Optimize your working model to refine, using the validation tools that are part of phenix.real_space_refine and phenix.polishit. Use any identify problem areas and using manual model building tools in Coot.

Advanced steps

Iteration of AlphaFold and model-building with experimental data

Combining information from AlphaFold and experimental data by refining the AlphaFold model and including your model building in processes and relaxing using other techniques. This process is what the phenix.predict_and_build procedure does, and it can be very powerful.

Structures with multiple chains

The phenix.predict_and_build tool can work with a structure with multiple chains, but you may want to run one chain at a time. This is because AlphaFold models are based on a single chain and may not be accurate when chains are in contact. If you do run all of the chain at a time the tool will try to build a model for each chain and place it in the unit cell, and then it will try to refine the model and combine the chain ensemble.

Boxing maps before rebuilding

For complex structures with many chains or with chains that contain DNA or RNA with long chains, starting can be very complicated and take a long time. In these cases it may be especially helpful to cut or mask the map if you are using phenix.predict_and_build. This can be done using phenix.boxmap or phenix.mask. Boxing the map can be helpful in any case, and it can be helpful in difficult situations. Cutting out the core NCS and then using phenix.ncs_ccf to find the NCS in the AlphaFold model and then using phenix.ncs_search_pdb_and_mtz to place the NCS in the cut out map can be very helpful in difficult situations. Using phenix.boxmap or phenix.mask to cut out the core NCS and then using phenix.ncs_ccf to find NCS in the AlphaFold model and then using phenix.ncs_search_pdb_and_mtz to place the NCS in the cut out map can be very helpful in difficult situations.

Background

Structure prediction software is now capable of generating models that are highly accurate over some or all of their complete sequences. These predictions often contain information that can be helpful in solving of crystallographic structures.

Contact distances in these predicted models in which all the residues have high confidence often will be very accurate. Even when the overall structure is not predicted well, the local structure of a domain may be predicted well enough to make molecular replacement, new molecule searches and phasing using manual model building tools to be more successful than without using the predicted models.

When using predicted models as a starting point for experimental structure determination, it can be helpful to:

- Make sure the model is in the right space group and in the correct hand.
- Correctly orient and position the model.

Once you have a reasonable model, you might try using the predicted model as a first, the most predicted models, but rather need to try to improve the confidence before. Then additionally try breaking the model into domains and using those as a starting point.

An important feature of recent predicted models is that they generally have very accurate sequence alignment information. Even when the overall structure is not predicted well, the local structure of a domain may be predicted well enough to make molecular replacement, new molecule searches and phasing using manual model building tools to be more successful than without using the predicted models. Even when the overall structure is not predicted well, the local structure of a domain may be predicted well enough to make molecular replacement, new molecule searches and phasing using manual model building tools to be more successful than without using the predicted models.

Since you have used Phenix tools to modify a predicted model based on experimental data you will need to identify whether the resulting models corresponding well enough to the experimental map or data. You will generally need to do some model building and refinement. Phenix has many tools for this, and the Xtriage tool is a good place to start.

You can also Rosetta the AlphaFold prediction using phenix.rosetta or you can use a cryo-em tool in AlphaFold (See the Documentation for running AlphaFold underneath)

Acknowledgements

Development of the Phenix AlphaFold tutorial (Jan 2, 2021), the Colaspa2 PDB-to-web prototype (Colaspa, Jan 1, 2021) and AlphaFold in Phenix (Jan 1, 2021) and sample decoys from ColabFold (Mirdita et al., 2021).

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amber

Phenix

Python-based Hierarchical Environment for Synopsis Bibliography

Running phenix.refine using Amber gradients

Contents

- Authors
- Theory and Background
- Running refinement with Phenix and Amber

Authors

Principal authors: Nigel W. Moriarty, Pavel Janowski, Ivo Nguyen & David A. Case

Contributors: Tom Darden, Kevin Shelley, Hanna Nilsson, Russ Walker (amber utilities is used in AmberPrep)

Theory and Background

Phenix is a software package for the automated solution and manipulation of Phenix crystallographic refinement and the Amber molecular mechanics force field for generating parameters. Amber contains facilities for construction and manipulation of molecular models, molecular dynamics and free energy calculations, and quantum mechanical and combined Hamiltonian MD simulations. Code in Amber's tleap and gaussian utilities interfaces are seamlessly integrated into Phenix and Phenix's Python-based hierarchical environment for synopsis bibliography (Phenix) has been added to Amber's tleap utility and AmberPrep. Phenix's Python-based hierarchical environment for synopsis bibliography (Phenix) has been added to Amber's tleap utility and AmberPrep.

Running refinement with Phenix and Amber

Phenix is a software package for the automated solution and manipulation of Phenix crystallographic refinement and the Amber molecular mechanics force field for generating parameters. Amber contains facilities for construction and manipulation of molecular models, molecular dynamics and free energy calculations, and quantum mechanical and combined Hamiltonian MD simulations. Code in Amber's tleap and gaussian utilities interfaces are seamlessly integrated into Phenix and Phenix's Python-based hierarchical environment for synopsis bibliography (Phenix) has been added to Amber's tleap utility and AmberPrep. Phenix's Python-based hierarchical environment for synopsis bibliography (Phenix) has been added to Amber's tleap utility and AmberPrep. To run Amber in Phenix, it needs to be installed and compiled. Phenix and Amber are installed in the directory /home/phenix/amber. Phenix finds the Amber executables and libraries by using the provided AmberPrep utility via the AmberPrep GUI or via the commandline:

```
phenix.amberprep
phenix.amberprep -h
phenix.amberprep -gui
```

which will generate four files:

```
amber.cmd
amber.log
amber.sh
amber.sh.o<jobid>
```

The first two are the Amber files and the last one is the PBS file that matches the new Amber files for given input. Phenix can be used to obtain Amber topology PLUS parm files(s) needed for input files. Refinement can be run as follows:

```
phenix.refine model.pdb data.mtz xray_data=fobs\*\*\*sigma,free=1\*\*\*xray_data=amber,ac=prmtop coordinates,ff=ff14ipbnd=amber,ac,ncf
phenix.refine -h amber
```

Here is list of keywords:

```
REQUIRED KEYWORDS:
  amber.ac  .ac - .ac reference with known geometry
            .ac - .ac reference with known geometry
            topology file name - obtained by the Amber topology file
                This is the prmtop file created by AmberPrep.
            parm file name - obtained by the Amber coordinate file
                This is the prmtop file created by AmberPrep.
            coordinates - obtained by the Amber coordinate file
                This is the crd file created by AmberPrep.
  optional keywords:
            ncf - .ncf - internal restraint factor between the x-ray and
                the force field energy terms. Default value is 0.0 if the x-ray and force
                fields. Other values may be given which have a default of 0.0 for the x-ray and force
                fields. Values must be > 0.0.

ADDITIONAL INFORMATION:
  amber.ac  .ac - .ac reference to energetically optimized coordinates using Amber's force field rather
            than the set of ideal & known restraints. This leads to models of improved quality. This minimization can be run
            using Amber.

  phenix.geometry.minimization.amber.ac_ac=1.amber.cmd=\"ac topology_file,name=amber,ac=1.prmtop coordinates,file_name=amber.ac=1.rst"

  2. AmberPrep contains additional options that the user may want to use. Run:

  phenix.amberprep -help.amber

  to view all options. Here is a list of the optional keywords:

  -help.amber  - type of energy minimization to perform. Possible options:
                 amber.ac  .ac - optimizes coordinates of all atoms using Amber's minimizer
                 amber.h   .prmtop - optimizes only hydrogen positions using Amber's minimizer (default)
                 phenix.ac - optimizes coordinates of all atoms using phenix minimizer
                 phenix.h  .prmtop - optimizes only hydrogen positions using phenix minimizer

  -chem  - chemical dictionary filter (TruePhenix, default False)

  -nmb  - use Amber's nmb force field instead of the default ff14ipbnd
                 Note: Amber's nmb force field is not supported by Amber developers as changed atoms and
                 atom types. It means the special account for the aromatic carbons attached to the
                 hydrogen atom in the ring is not taken into account. Also, the hydrogen atoms in the
                 refinement where using the classical charge (really force field) but used are free to experiment
                 with charge and mass.
```

3. Refinement with Amber currently has several limitations. All atoms must be explicitely modelled and there can be no gaps in the peptide or nucleic acid backbone. If hydrogen atoms are missing, they will be added. Currently, Amber's tleap utility is used to add hydrogens. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported. Solvation or PBC are not supported. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported.

4. Metal containing ligands are not supported by Amber.

5. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported.

6. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported.

FOR BUSINESS CARDS:

1. To use Phenix instead of Amber for geometry calculation, use ac4_engine=ccp4 keyword for phenix.refine. The default is ac4_engine=amber.

2. phenix.refine and Amber also has a limited ncs. Phenix generates .ncs extensions (refinement the x-ray term is not yet supported). Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported.

3. The default value of charge for the charge of the ligand is 0.0 for the Amber parm file generation. The default value of charge for the charge of the ligand is 0.0 for the Amber parm file generation. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported. Phenix's Amber interface does not yet support the use of Amber's sander utility for molecular dynamics. Solvation or PBC are not supported.

4. Phenix's Amber interface performs several important actions to prepare files for refinement with Phenix and Amber

Phenix *Python based Hierarchical Environment for Integrated Xtallography*

Analysing alternative conformations matching a map with analysis_alt_conf

Author(s)

Pavel Afonine, Oleg Sobolev, Tom Terwilliger

Purpose

The purpose of analysis_alt_conf is to analyse alternative conformations (focusing on side chains) for a structure against a given reflection data.

The analysis tool is a phenix.clash type tool, analyse conformations present in two structures, identifying which one is better and which one is clashy or bonkers.

How analysis_alt_conf works:

System Message: WARNING/3 (`/usr/lpp`, **line 21**)

Title underline too short.

```
Map analysis_alt_conf model
```

The tool first superposes all models that are supplied. Then it analyses the unique residue conformations in each model, identifying those that are different and those that are the same. Residues are considered all (C) or (N) atoms are considered for clash conformer, those with a larger clash are considered offended.

If there are two models supplied, the tool then compares the unique conformers in the first and second models, and finds those that are better in the second model (clash wise) and those that are better (clash wise) in the first model.

Examples

Standard run of analysis_alt_conf:

System Message: WARNING/3 (`/usr/lpp`, **line 30**)

Title underline too short.

```
Example run of analysis_alt_conf:
```

Running analysis_alt_conf in CCP4 shell, from the command line one can type:

```
phenix.analysis_alt_conf model_1.pdb model_2.pdb
```

where model_1.pdb is the model you would like to use as a starting point and other_model.pdb is an optional second model.

Possible Problems

The analysis tool analyses alternative side chain conformers, not main chain. If you main chain has substantial alternative conformations (not just slight adjustments) to match the side chain conformers, you will get misleading results.

Literature

Additional information

List of all available keywords

```
ALL_KEYS = None                          ALL_KEYS, A PRINTED ARG, TOP LEVEL OF COMMAND TLVS
  ALL_OUT = None
    model = None                         input model
analysis_alt_conf
  output_prefix = model + '_A'           Prefixes that between contains, we shown in chosen dirfor to this
    model_alt_conf = None                Output alternative conformers
    model_alt_diff = None + '_diff'      Output alternative conformers, that take clashed parts
                                         Output difference between models
out                                      Optionally parameter required for output directory
    output_dir = None
```

Phenix *Python-based Hierarchical Environment for Integrated Nanosystems*

Analyzing the anomalous signal in a SAD dataset with anomalous_signal

Author(s)

P. Afonine, Joseph Ton Terwilliger

Purpose

This program is a tool for estimating the anomalous signal in a SAD experiment and for predicting whether phasing will be successful in solve the structure. This tool normally is used in conjunction with phenix.xtriage.

Note: this assessment (predicting the experiment) will scale, phase, and/or locate the overlapped data and also perform phasing (optional).

Usage

How anomalous_signal works:

- Input anomalous data and optional sequence data, two half-dataset files with scaled anomalous data, and optional model file (PDB or CIF) to compute the expected anomalous signal.
- anomalous_signal will calculate the anomalous signal in your dataset from (1) the half-dataset anomalous differences, and (2) the expected anomalous signal from your model and your sequence (if supplied).
- anomalous_signal will also provide the probability that you can solve the dataset using likelihood-based methods (SHELX, Phaser, and others) and the resolution at which this is most likely.
- The two final plots (ccc_experiment and anomalous_signal) estimate the probabilities that you can solve the structure and the resolution at which this is most likely. These plots are based on a comparison of your data with the same resolution range in a large database that we are drawing from to scale and to estimate the probabilities.

Output from anomalous_signal

anomalous_signal provides a summary of the scale, measurement errors, and half-dataset correlations in your data, and estimates the probability of success of solving the structure and estimated figures of merit of phasing. Here is an example:

```
                    Cycle 1 of target is this dataset
                    ---------------------------------

                    ------------------------------------------------------
                    |  Resolution range   |  Number  |  Average  |  Average  |
                    |  low      high      |  of data |  sigma    |  signal   |
                    ------------------------------------------------------
                    |  10.00    3.00      |   1000   |   0.000   |   0.000   |
                    |  3.00     2.50      |   1000   |   0.000   |   0.000   |
                    |  2.50     2.00      |   1000   |   0.000   |   0.000   |
                    |  2.00     1.70      |   1000   |   0.000   |   0.000   |
                    |  1.70     1.50      |   1000   |   0.000   |   0.000   |
                    |  1.50     1.40      |   1000   |   0.000   |   0.000   |
                    |  1.40     1.30      |   1000   |   0.000   |   0.000   |
                    |  1.30     1.20      |   1000   |   0.000   |   0.000   |
                    |  1.20     1.10      |   1000   |   0.000   |   0.000   |
                    |  1.10     1.00      |   1000   |   0.000   |   0.000   |
                    ------------------------------------------------------
                    Overall                 10000      0.000       0.000
```

Applying NCS to a molecule to generate all NCS copies with apply_ncs

Author(s)

- Jack Dai, Eric Terwilliger

Purpose

If you have a single copy of your molecule present in the crystal and you have a set of NCS operators defined in an ncs.ncs.spec file (such as from AutoNCS or phenix.find_ncs), you can apply the operators to your molecule to generate all NCS copies in the crystal. This is useful for visualizing the NCS copies in the crystal, or for generating a complete model of the crystal from which to run other phenix programs (for example, phenix.refine ncs=true requires a complete model of the crystal, not just one NCS copy).

Usage

How apply_ncs works:

apply_ncs processes PDB files and expanding it with one copy of your molecule shifted to cover your ncs.ncs.spec and ncs.ncs.mtrix operators. It then writes out the expanded PDB file. Optionally, it can also write out a new ncs.ncs.spec file with the expanded model and updated operators. Again, such an expanded model and NCS operator set can be used in other phenix programs, for example, phenix.refine ncs=true requires a complete model of the crystal and corresponding to your input molecule.

apply_ncs can also write out a new ncs.ncs.mtrix file for your molecule to mtrixncs.n, and then use all the NCS operators to transform molecule.n to match NCS copy.

Output files from apply_ncs

apply_ncs.pdb: A PDB file with your input molecule placed at all the NCS related positions in your structure

Examples

Standard run of apply_ncs:

Running apply_ncs is easy. From the command line you can type:

```
phenix.apply_ncs model.pdb ncs.ncs.spec
```

If apply_ncs chooses the wrong NCS to match up to your input molecule, you can tell it which one your input molecule is with instead, as:

```
phenix.apply_ncs model.pdb ncs.ncs.spec mtrix=2
```

apply_ncs will then assume that you are applying ncs copy 2.

Possible Problems

Specific limitations and problems:

Literature

Additional information

The documentation for PhenoLib describes how to find and apply NCS information for helical arrays, point-group symmetry, and non-crystallographic symmetry.

List of all available keywords

```
apply_ncs (.phil
  model = None                      PDB FILE TO USE
  ncs_spec = None                   NCS SPEC FILE
  mtrix = None                      Input NCS file
                                    Optional file containing ncs in mtrix format (ncs.mtrix
                                    or ncs.ncs.mtrix) to use instead of ncs in ncs_spec file
                                    (default: use ncs in ncs_spec file). Note: if ncs_spec
                                    is not given, ncs will be read from mtrix file. Note:
                                    if ncs_spec is given and mtrix is given, ncs will be
                                    read from ncs_spec file and mtrix will be ignored.
                                    Note: if ncs_spec is given and mtrix is given and
                                    ncs_spec file has no ncs, then ncs will be read from
                                    mtrix file if mtrix=1 is specified.
                                    Note: if ncs_spec is given and mtrix is given and
                                    ncs_spec file has no ncs, then ncs will be read from
                                    mtrix file if mtrix=1 is specified.
                                    Note: if ncs_spec is given and mtrix is given and
                                    ncs_spec file has no ncs, then ncs will be read from
                                    mtrix file if mtrix=1 is specified.
  ncs_id = None                     Input NCS file
  output_file = None                Output PDB file
  output_ncs_spec = None            Output NCS spec file
  write_ncs_spec_file = False       Write out ncs_spec file
  write_mtrix_file = False          Write out mtrix file
  write_ncs_spec_and_mtrix_files = False
                                    Write out ncs_spec and mtrix files
  write_expanded_ncs_spec_file = False
                                    Write out ncs_spec file with expanded ncs
  write_expanded_mtrix_file = False
                                    Write out mtrix file with expanded ncs
  write_ncs_chains = False          Write out ncs chains
  write_ncs_chains_separately = False
                                    Write out ncs chains separately
  write_ncs_chains_separately_prefix = None
                                    Prefix for ncs chains separately
  write_ncs_chains_separately_suffix = None
                                    Suffix for ncs chains separately
  write_ncs_chains_separately_start_with_1 = True
                                    Start ncs chains separately with 1
  write_ncs_chains_separately_start_with_1_for_each_chain
                                    = True
                                    Start ncs chains separately with 1 for each chain
  write_ncs_chains_separately_keep_original_chain_ids
                                    = False
                                    Keep original chain ids in ncs chains
  ncs
    ncs_info
      ncs_group_id = None           ncs group id
      center_1 = None               Center of first ncs group (optional) (default: use
                                    center of first ncs group)
      center_2 = None               Center of second ncs group (optional) (default: use
                                    center of second ncs group)
      rotation = None               Rotation matrix (optional) (default: use rotation
                                    matrix from ncs group)
      translation = None            Translation vector (optional) (default: use
                                    translation vector from ncs group)
      apply_ncs = None              Apply ncs to this ncs group (default: apply ncs to
                                    all ncs groups)
      is_ncs_to_cart = False        Is ncs in cartesian coordinates (default: ncs in
                                    fractional coordinates)
      apply_ncs_operators_only = False
                                    Apply ncs to the NCS operators directly (a rare event
                                    that you would want to do this, for example, if you
                                    have ncs that is based on NCS operators in their own
                                    right)
      ncs_chains = None             Use the chains in this ncs group
      ncs_chains_exclude = None     Do not use the chains in this ncs group
      ncs_chains_exclude_selection = None
                                    Do not use the chains in this ncs group (selection)
      apply_ncs_operators_only_to_selection
                                    = False
                                    Apply ncs to the NCS operators directly to the chains
                                    in this selection (a rare event that you would want
                                    to do this, for example, if you have ncs that is
                                    based on NCS operators in their own right)
      ncs_chains_for_ncs_operators_only = None
                                    Use the chains in this ncs group for ncs operators
                                    only (a rare event that you would want to do this,
                                    for example, if you have ncs that is based on NCS
                                    operators in their own right)
      ncs_chains_for_ncs_operators_only_selection
                                    = None
                                    Use the chains in this ncs group for ncs operators
                                    only (selection) (a rare event that you would want to
                                    do this, for example, if you have ncs that is based
                                    on NCS operators in their own right)
      apply_ncs_only_if_ncs_chains_present
                                    = False
                                    Apply ncs only if ncs chains present (default: apply
                                    ncs to all ncs groups)
  optional
    verbose = False                 Verbose output
    debug = False                   Debug output
    debug = False                   Debugging output
    file_name = None                Input PDB file (alternative input)
    write_log_file = None           Write log file
                                    Write log file (default: write log file to
                                    output_dir/output_prefix.log) (if output_prefix is
                                    not specified, output_prefix defaults to "phenix")
                                    (default: write log file to current directory)
```

assign_sequence

Phonis

Python Issue Resolution Framework for Bioinformatic Workflows

Sequence assignment and linkage of substructuring segments with assign_sequence

Author(s)

J. Kniel, Johannes Tom Renzelmann

Purpose

You can start work on an unlinked sequence assignment of a model that you have already built with substructuring segments. The assignment of the segments to the sequence is then carried out automatically and subsequently linked to the substructuring segments. This is the task of the assign_sequence command. The sequence can be read in beforehand or directly when the command is called.

assign_sequence is a command line tool for generating pairwise sequence assignments for a model and a map. The sequence assignments are written to a file in the Clustal format and the segments in the map are linked to the corresponding sequences. Since a multiple sequence alignment consists of a sequence and pairwise sequence assignments, assign_sequence can use the PIL input map library to convert sequences that are required by a tool.

Note: assign_sequence is designed for so-called alignment-based methods in which sequence A is aligned against a reference sequence B. The reference sequence B is the sequence of the target structure. If you want to create an input for several or no alignments, or if you know that it is complicated, note the sequence assignment for multiple sequences in the Clustal format manually.

NOTE: assign_sequence is normally called from phenis-align, plus tools that you can run in interactively if you want.

Usage

Have assign_sequence works:

The starting point for assign_sequence is a set of segments of structure read in from the input model. assign_sequence then generates pairwise sequence assignments for the segments and links the segments to each sequence. Then assign_sequence writes pairwise combinations of alignments of all the segments to the output file in the Clustal format. The segments are linked to the sequences in the output map. For further PIL tools, and with the generation and alignment between ends of the segments.

Segment assignment

assign_sequence can read the sequence in two compatibility modes: assign_sequence creates two sequence assignments of each possible pairs which are stored pairwise in the input model. Segments that are particular sequence assignments are linked to the sequence. The segments are then assigned to the sequence. Multiple sequences, of which sequences have a number of segments, with a number of possible combinations of segments. Segments are linked to the sequence. Segments are linked to the sequence. Segments are linked to the sequence. Segments are linked to the sequence.

Segment assignment

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Segment assignment

Generating sequence alignments and connections

Generating sequence alignments and connections: assign_sequence generates pairwise sequence assignments. Often these are known and aligned sequences generated by separate alignment tools. Sometimes the sequence assignments are generated by assign_sequence. Sometimes the sequence assignments are generated by assign_sequence. Sometimes the possible sequence assignment of each subsequent segment is stored for compatibility with the existing sequence assignment. Segments are linked to the sequence. Segments are linked to the sequence. Segments are linked to the sequence. Segments are linked to the sequence

```
check_kv_size_with_prefixes : bool
                              True to verify RDB keysizes when loading the RDB file accordingly.
                              Prefixes are used to partition the keyspace by key prefix.

find_big_keysizes : bool      True to output keysizes histograms (every known type and
                              cardinality) at the end of the RDB file loading.

print_big_keysizes : bool     True to output top keysizes (of any type) over the
                              pre-configured limits.

write_freq_histogram : bool   True to output keysizes histograms exclusively at exact fixed
                              intervals (the interval is hard-coded to 1 million keys).
                              Useful when trying to chart RDB keysizes growth in time without
                              being affected by the dynamic nature of the keyspace.

dir_to_flush : bytes          For AOF compatibility. Redis will fsync AOF manifest changes
                              to this directory.

                              Note: Redis-RDB-check does not fsync anything to disk, since
                              it is a read-only tool. However, it may be ran against a
                              directory which is used by a running Redis instance.

keep_connections : bool       Only in this version of the parser and RDB-check, it
                              keeps the connection open after the initial handshake.
                              Used to test support for persistent connections.

                              Note: in this version of the parser and redis-check-rdb, the
                              connection will be closed if the server sends any data
                              (which is not the expected response to the initial handshake).
                              This is to ensure that the parsing code does not read
                              unexpected data from the connection.

include_rdb_checksum_in_hmac : bool
                              When enabled, the checksum of the RDB is included in payload with
                              the HMAC.

psync_replid_len : int        Length of the replication id in the psync handshake.
                              Usually 40.

psync_replid_is_all_zeros : bool
                              If true, the replication id in the psync handshake is
                              all zeros (indicating a request for a full sync).

remote_replication_offset : int
                              The initial replication offset to ask for in the psync handshake.
                              Ignored if the replication id is all zeros.

replica_ping_period : int     If > 0, then this is the ping frequency in replication keepalive
                              packets (in seconds). Ignored if the replication id is all zeros.

discard_rdb_payload : bool    If true, then this is the response numbers expected in response as
                              part of the handshake.

allow_fake_connections : bool If enabled, expect to successfully pass the handshake (the
                              server will send the expected response to the handshake).
                              Otherwise, close the connection as soon as the handshake
                              starts (the server will send a wrong response).

replica_ack_period : int      Send REPLCONF ACK every this number of seconds.

dump_payload_length : int     Deliberately lie about the payload length.

dump_payload_checksum : int   Deliberately lie about the checksum.

n_clients : int               Number of fake clients to spin.

max_inline_bytes_client_buffer : int
                              Maximum number of inline bytes allowed length on fake clients.
                              Used to test the "client output buffer limit" feature. Replying
                              to the ping command with a bigger value than this limit
                              will trigger the client to be disconnected.

command_delay : float         Delay between replicating each command.
                              Used to test the "client output buffer limit" feature.

send_interval : int           Delay between sending every chunk of data.
                              Used to test the "client output buffer limit" feature.

dump_to_aof_format : bool     Instead of sending the RDB to the server, write it to stdout
                              in a RESP protocol format (to be ran into redis-cli).

dump_to_aof_format_timestamp : bool
                              When dump_to_aof_format is on, if this flag is set, the
                              generated AOF will contain timestamp annotations.

dump_commands : bool          Dump the received commands to stdout.

cluster_slots_bitmapsize : int
                              Size of the cluster slots bitmap.
                              Usually 16384 (the number of hash slots in the cluster).

dump_bitmap : bool            Dump the received cluster slots bitmap to stdout.

dump_slots : bool             Dump the received cluster slots to stdout.

dump_sequence_file : bytes    If not empty, then dump the received replicated command sequence
                              into this file.

dump_sequence_overflow_file : bytes
                              If not empty, then dump the received replicated command sequence
                              into this file, if the sequence file reaches its limit.

sequence_file_size_limit : int
                              Maximum size of the sequence file (in bytes).
                              Ignored if the sequence file is empty.

sequence_file_offset : int    Start offset in the sequence file.
                              Ignored if the sequence file is empty.

sequence_file_repeat : int    Number of times to repeat the sequence file.
                              Ignored if the sequence file is empty.

sequence_file_no_wait : bool  If true, then ignore wait commands in the sequence file.
                              Ignored if the sequence file is empty.

sequence_file_replconf_ack : bool
                              Convert all sequence commands to REPLCONF ACK.
                              Ignored if the sequence file is empty.

sequence_file_ignore_ping : bool
                              Ignore PING in the sequence file.
                              Ignored if the sequence file is empty.

dump_rdb_to_aof_file_path : bytes
                              Dump the RDB to this file in AOF format.

rdb_checksum_file_path : bytes
                              Write checksum of the dump into this file.

rdb_checksum
    crc64 : int               Received checksum.
    crc64_calc : int          Calculated checksum.

rdb_header
    magic : bytes             Magic number.
    rdb_version : int         RDB version.

rdb_footer
    crc64 : int               Received checksum.
    crc64_calc : int          Calculated checksum.

rdb_aux_field_key : bytes     Received auxiliary key.

rdb_aux_field_value : bytes   Received auxiliary value.

rdb_db_number : int           Current database number.

rdb_resize_db_hash_table_size : int
                              Received hash table size for the current database.

rdb_resize_db_expire_hash_table_size : int
                              Received expire hash table size for the current database.

rdb_module_aux_field_name : bytes
                              Module name.

rdb_module_aux_field_value : bytes
                              Module value.

rdb_module_aux_field_opcode : int
                              Module opcode.

rdb_module_aux_field_when : int
                              Module when.

rdb_module_aux_field_sint : int
                              Module signed integer.

rdb_module_aux_field_uint : int
                              Module unsigned integer.

rdb_module_aux_field_raw : bytes
                              Module raw.

rdb_module_aux_field_end_of_aux : bool
                              Module end of auxiliary.

rdb_module_aux_field_error : bool
                              Module error.

rdb_module_aux_field_skip : bool
                              Module skip.

rdb_module_aux_field_data : bytes
                              Module data.

rdb_module_aux_field_eof : int
                              Module eof.

rdb_module_aux_field_unknown : bytes
                              Module unknown.

rdb_module_aux_field_unknown_type : int
                              Module unknown type.

rdb_module_aux_field_unknown_when : int
                              Module unknown when.

rdb_module_aux_field_unknown_data : bytes
                              Module unknown data.

rdb_module_aux_field_unknown_eof : int
                              Module unknown eof.

rdb_module_aux_field_unknown_sint : int
                              Module unknown signed integer.

rdb_module_aux_field_unknown_uint : int
                              Module unknown unsigned integer.

rdb_module_aux_field_unknown_raw : bytes
                              Module unknown raw.

rdb_module_aux_field_unknown_end_of_aux : bool
                              Module unknown end of auxiliary.

rdb_module_aux_field_unknown_error : bool
                              Module unknown error.

rdb_module_aux_field_unknown_skip : bool
                              Module unknown skip
```

atom_selections

Phenix *Python based Hierarchical Environment for Integrated Crystallography*

The Phenix atom selection syntax

Contents

- Introduction
- Video Tutorial
- Examples for selection expressions
- Grammar selection
- Grammar parameters

Introduction

Many of the programs in Phenix, and phenix.refine in particular, allow (or require) you to specify selections of atoms in a simple common grammar for:

- Selections for atomic model manipulation and ligand fitting refinement groups
- Selections for atomic value annotation in Xtriage reflections
- Selections for atomic model validation
- Subset of atoms to modify properties for CC-Omitmap
- Selections for atomic model comparison in LSQ

All of these processes are defined using a common atomic entities to which is used in CIF or PDB. The syntax for selecting these atoms is based on the Python based Hierarchical Environment for Integrated Crystallography (PHENIX) syntax and simplified versions of the use of simple boolean statements (and, or, or only)

Video Tutorial

The Tutorial video is similar to the Phenix Starter tutorial and covers the following topics:

- Basic syntax
- Simple atom selection syntax
- Examples for selection expressions
- Advanced syntax (boolean operations and other selection)

Examples for selection expressions

All atoms

```
all
```

All C alpha atoms (not case sensitive)

```
name ca
```

All atoms with X in the name (* is a wildcard character)

```
name *x*
```

Atoms canoe with * (backslash disables wildcard function)

```
name *can\*
```

All atoms in A' conformation

```
altloc a'
```

Atom name with spaces

```
name " h"
```

Atom name with primes don't necessarily have to be quoted

```
name o5*
```

Boolean "and", "or", and "not"

```
chain A and name ca
chain A or chain B or chain C or name c or name n
chain A and not chain B
chain A and not name ca or chain B or chain C
```

Note that in the last example, the selection is ambiguous, parenthesis may be required to indicate which boolean applies. The first example above selects for all atoms with the specified name in atoms matching chain A or chain B or chain C. The last example selects atoms for all chains and the specified name in atoms matching chain A but not chain B.

```
chain A or chain B or chain C and name ca
chain A and not chain B or chain C and name c
```

A set-valued select 1 alpha atom in A, plus all atoms name C, N, or O regardless of residue name.

Also note that the outcome of boolean expression can be somewhat different from what one may expect. Consider the following example. Suppose that the PDB contains chain B but not chain C. The following two selections are identical:

```
chain A or chain B or chain C
```

because suitable residues from residue name ALA or ILU (in the contrary, selection

```
residue ala or resseq 1c
```

will result in empty selection because there is no residue that can satisfy both conditions simultaneously.

A single residue by number

```
resseq 1
```

Note that if there are several chains containing residue number 100, all of them will be selected. To be more specific, one may specify the chain of particular chain:

```
chain A and resseq 100
```

this will select residue 100 only in chain A.

A range of residues

```
resseq 1:10
```

Selection includes residues falling within the range, independent of their order in the PDB file. The numbering must be ascending. resseq 10:1 will not work.

Insertion codes

Residues with insertion code resseq number (resseq with the insertion code (icode) thus the following selections are identical:

```
resseq 5a
icode a and resseq 5
```

Or in Chain

```
chain A or chain B
```

Specifying ordered range of residues

Residues are ordered in the PDB file in Phenix. It may be important to specify a numerical range of resseq attributes. This is especially the case when the residue numbering is not continuous and ascending, which is common in the PDB. In this case, one may specify the range of residues in the selection using the resseq or resnum keywords for their numerical number and insertion code, using the icode keyword.

```
resseq 1:10 and not resseq 5:8
```

In this case, the residues will be examined in the order that they appear in the PDB file, and every atom falling between the specified ranges will be included. This is the only situation where the ordering of atoms is important in atom selection.

B-factors and occupancies

Sky has the ability store based on their numerical properties:

```
bfactor 0 -
bfactor 0 - 10
bfactor 10 -
occupancy 0 -
occupancy 0 - 1
occupancy 1 -
```

Alternates

A few additional keywords are supported:

```
alternate A
alternate B
alternate
altloc A
```

These are simple exactly hydrogen atoms, water molecules (detected by residue name), common amino and nucleic acid atoms (detected by atom name), respectively.

Selecting on atoms

```
name CA
```

The syntax for the atom selection is less rich in the GUI, but still supports one or more. Note, the treatment of this differs depending on how the atom selection will be used. For grid selections, base is interpreted in two ways: as a single letter, or as a comma-separated list of single letters. Selecting on base "A" will select all A-form alternates, leaving the selection as is, but will select a new alternate/occupancy being alternate/occupancy 1 if the selection is empty. Selecting on base "A,B" will select A and B alternates.

Graphical selection

In the pulldown menu Grid, any atom selection can be visualized if you have a suitable graphics card and OpenGL installed. Sky will then show the selected atoms in a different color, and allow selection by clicking the "Selection" button next to any atom selection field. Depending on the size of your structure, it may take a few seconds for Sky to calculate the atomic connectivity. The current selection, if any, will be highlighted.

The View grid button opens a window that allows you to type in selections and immediately visualize the results, without having to open the selection dialog. Sky will show the selected atoms in a different color. Clicking the button left open in the selection dialog works similar in intent. However, we recommend that you leave the View grid button open, and use the selection dialog only for complex selections, or when you want to keep the last selection/alternate in the appropriate slot.

Sky remembers the last 10 selections. Clicking on the Undo button, clicking a different "Recent" button and transfer control of the display (the mouse and keyboard) to Sky. Sky will then show the atoms more and less distinct another to allow you to see the difference between the current and the selected one.

"Smart" selections

In some situations (pertaining to residue-active and Ramachandran) the geometry mainterm information is used to determine the selection:

```
residue and backbone
residue and sidechain
residue and ca
residue and ca and sidechain
residue and ca and sidechain or carbon
residue and ca and sidechain or carbon or nitrogen
```

Note however that these options cannot be visually selected in the Pharos GUI at present, and they may not be recognized by all programs.

Phenix | *Action:Input*/*Restriction*/*Parameter*/*Output*/*Keyword*:

Auto-sharpen (deprecated, use MapSharpening)

Author(s):

- Andre Jurgens: Tom Terwilliger

Purpose

This module auto_sharpen will automatically identify optimal sharpening/blurring/map adjustment for the input map based on the estimated resolution of the map.

Video Tutorial:

The tutorial video is available on the Phenix YouTube channel and covers the following topics:

- Map sharpening
- Automatic sharpening of cryo-EM maps, by model vs by FSC

GUI

A graphical user interface is available.

Usage

How auto_sharpen works:

Auto-sharpen adjusts the resolution dependence of the map to maximize the clarity of the map. You can choose between two methods: sharpening to maximize the correlation of the map with a model, or by FSC.

The auto-sharpen tool works best at resolutions of about 3.5 A or better. At lower resolutions it may be unable to distinguish variations in the quality of the map as the sharpening is varied.

The tool can optionally also sharpen the map to emphasize the connectivity of the map.

The sharpening procedure is a combination of the surface sharpening of Terwilliger et al. (2007) and a particular treatment of the number of distinct regions estimated by the CRS (Wilkinson et al. (2009)). The sharpening is carried out by a combination of a resolution-dependent B-factor and a surface-based sharpening. The surface-based sharpening is carried out by applying a local B-factor that is a function of the distance from the surface. The surface is defined by a particular value of region-connectivity.

Several resolution-dependent functions are tested, and the one that gives the best adjusted surface area (or connectivity) is used. The resolution-dependent functions are defined by a set of Fourier coefficients and these coefficients are then adjusted, keeping the phases constant. The available functions for modifying the amplitudes are:

```
  No sharpening (map_to_info_mc)
  Sharpening to a target amplitude versus resolution (map_q_target)
  Sharpening to maximize the surface connectivity (surface_q_mc)
  Sharpening to maximize the surface-to-volume ratio (surface_q_ratio)
  Sharpening to maximize the connectivity (connectivity_q_mc)
  Sharpening to maximize the connectivity and surface (connectivity_surface_q_mc)
  Sharpening to maximize the connectivity and surface (connectivity_surface_q_mc)
  Sharpening to maximize the connectivity and surface (connectivity_surface_q_mc)
  Sharpening to maximize the connectivity and surface (connectivity_surface_q_mc)
```

```
Structure-dependent sharpening factor with Fermi weightings
Structure-dependent sharpening factor with Gaussian weighting
Structure-dependent sharpening factor with Gaussian weighting for
Sigma-A estimation using Gaussian target function
Sigma-A estimation using Gaussian target function for
Sigma-A estimation using Gaussian target function for
Sigma-A estimation using Gaussian target function for
```

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Specifying other parameters
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Specifying other parameters
Specifying other parameters
Specifying other

and the removed residues will be in the file:

```
./ambdock_results_removed.pdb
```

You can update just the score parts of your model by adding dock2score flag. Because dock2score flag will recalculate the interface residues, it will also update the interface residues in the output PDB file. Without dock2score flag, only the score parts will be updated and the interface residues will remain unchanged.

Note that since this is optional, if you do not provide it then it will default to not updating the score parts of your model.

Create 20 very good rebuilt models that are different as possible

```
python $AMBDOCK_DIR/ambdock.py -m model.pdb -p protein.pdb -r 20
-d dock.pdb -s dock.sc -n 20 -o rebuilt.pdb
```

This command will ask for 20 rebuilt models (-n 20) based on the input PDB file of the rebuilt docks. The procedure is similar to the above example except that the -r option is used to ask for 20 rebuilt models. The -r option is used to specify the number of rebuilt models to be produced. The particular flavor of Rosetta rebuild is that they can be very accurate but very different from the original model. This is because Rosetta rebuilds the entire model from scratch. The -r option is also used to keep only the different rebuilt models. Rosetta rebuilds models that are very different from the original model but it also rebuilds models that are very similar to the original model. The -r option will discard models that are too close to a special reference (0.45 RMS by default). The reference is the original model plus all previously rebuilt models. The -r option will keep only the rebuilt models that are different enough from the original model and from each other. The -r option is used to make sure that the rebuilt models are different from each other. The -r option is also used to make sure that the rebuilt models are different from the original model. The -r option is also used to make sure that the rebuilt models are different from each other. The -r option is also used to make sure that the rebuilt models are different from each other. The -r option is also used to make sure that the rebuilt models are different from each other

```
CONTROL_BATCH_SELECT=1
                    # Select with the keyboard and mouse.
                    # Select with the keyboard only.
                    # Select with the keyboard and mouse and use the keyboard
                    # to move the selection. Pressing Shift or Ctrl toggles
                    # the selection. Pressing Alt toggles between the two
                    # modes. Pressing Alt twice toggles the selection of the
                    # current item. Pressing Alt twice and then Shift
                    # toggles the selection of a range of items.
CHUNK_PARSE_QUOTE_CHAR="'"
                    # The character used to quote strings and characters
                    # in the chunk parser.
CONTROL_SCROLL_1=1  # Scroll by the number of lines in the scroll field.
                    # Scroll by the number of pixels in the scroll field.
                    # Scroll by the number of pixels in the scroll field
                    # times the number of lines in the scroll field.
                    # Scroll by the number of pixels in the scroll field
                    # times the number of lines in the scroll field and
                    # invert the direction of scrolling.
                    # Scroll by the number of pixels in the scroll field
                    # times the number of lines in the scroll field and
                    # invert the direction of scrolling if the mouse
                    # cursor is in the upper half of the screen
```

Automated molecular replacement with AutoMR

Author(s)

- Pieter Meiring | Tesla Solutions | PhD and Lecturer | Member
- Jacques Theron | Tesla Solutions | Senior Lecturer | Doctor | Member
- Andrew Mkhize | Tesla Solutions | Senior Lecturer | Doctor | Member
- Jabulani Khoza | Tesla Solutions | Lecturer | Member

Purpose

Purpose of the AutoMR Wizard

The AutoMR Wizard provides a convenient interface to Phaser molecular replacement and feeds the results of molecular replacement directly into the AutoBuild Wizard for automated model rebuilding.

Phaser molecular replacement is a powerful method for solving the phase problem using a search model or models, with the probability of the search models first and foremost in the mind.

Usage

The AutoMR wizard has been deprecated and is no longer available in the Phenix GUI, but it may still be run from the command line, and from automation. The AMR wizard provides several options that may still find help documented from the user manual PDF or Phenix Phaser. Some of them is not a Phaser.

Summary of inputs and outputs for AutoMR

Input data file: This file can be in most any format, but most contain either amplitudes or intensities and phases. The program will try to guess what is in the file and what to do with it. Phenix will convert intensities to amplitudes if necessary. Phenix will also try to find the appropriate data set in the file if there are more than one. Phenix will also convert phases to Hendrickson-Lattman coefficients if necessary. Phenix will try to find a suitable anomalous scattering set if anomalous data are present. Phenix will try to find a suitable free-R set if one is not specified.

Contents of the asymmetric unit: PHASER needs to know what the total mass in the asymmetric unit is. In most cases, this information is provided in the form of a sequence file. Phenix can also estimate the total mass of the asymmetric unit from the sequence or molecular weight. Alternatively, one can specify the Matthews coefficient and the number of copies of the asymmetric unit.

Space group to search: You can request that all space groups with the same point group as the one you start with be searched. Phenix will also try all chirals if you select the option that lists space group with the same Laue class. Phenix will also try all chirals.

Ensembles to search for: AutoMR looks up a model by finding a set of pdbid sequence and orientation of sub-ensembles. Phenix will also search for homologous structures. Phenix will also search for models in the current directory of the asymmetric unit and find and a standard solution is obtained. You can specify the number of copies of each ensemble to be found. Phenix will also try to find a suitable ensemble. Phenix will also try to find a suitable ensemble. Phenix will also try to find a suitable ensemble

autosol

Phenix

Action-based Structural Biology ⊗ *Phenomics for Structural Biology*

Automated Structure Solution using Autosol

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Authors

Tom Terwilliger Peter Zwart Nigel Bunkoczi Airlie McCoy Randy Read Isaac Vedovato Ralf Grosse-Kunstleve Ann Richardson Gabor Bunkoczi, Ronald Beck Thomas Waldo Daniel Waterman Paul Adams Nathaniel Echols

Purpose

The Autosol Wizard uses HYSS, SOLVE, RESOLVE, phenix.refine and phenix.refine to solve a structure and produce an initial model and map. The Autosol Wizard can be run in a fully automated mode or can be run interactively with the user specifying the number of heavy-atom sites, the number of cycles of phasing and density modification, and the number of cycles of refinement and NCS identification and NCS averaging.

Usage

The Autosol Wizard can be run from the PHENIX GUI. Form the command line, and from phenix.hyss. All Autosol Wizards can be run from the command line using the command phenix.autosol. The command line version of the Autosol Wizards for details of how to run a Wizard. The command line version will by default ask, except for MR and MRSAD, for the number of sites, the number of cycles of phasing and density modification, and the number of cycles of refinement and NCS identification and NCS averaging. The command line version will also by default ask for the name of a sequence file and for the name of a PDB file with a model to be used for NCS.

How the Autosol Wizard works

The main task for the Autosol Wizard which will be described below. They are: Setting up inputs, Analysing and scaling the data, Finding heavy-atom (anomalously-scattering atom) sites, Scoring and refinement of heavy-atom sites, Phasing, Density modification, Including NCS averaging, and Preliminary model building and refinement. The Autosol Wizard can be run in a fully automated mode or can be run interactively with the user specifying the number of heavy-atom sites, the number of cycles of phasing and density modification, and the number of cycles of refinement and NCS identification and NCS averaging.

Setting up inputs

The Autosol Wizard expects the following basic information:

- a sequence file for the macromolecule
- a reflection file with data for the Wizard to use
- a PDB file with a model for the macromolecule (optional)
- how many sites to look for in the data (or none, to skip this step)
- a PDB file with a model for the heavy-atom substructure (optional, if substructure is known)

The Autosol Wizard can also use information about the number of copies of the macromolecule in the asymmetric unit (optional) and information about the number of copies of the heavy-atom substructure (optional).

You can also specify many other parameters including resolution, number of sites, solvent fraction, and a variety of parameters that control the operation of the Wizard. The Wizard will use default values for all parameters if you do not specify them.

Quickfile formats in Autosol

Autosol can accept the following formats of data:

- reflections in Quickfile format (.hkl)
- sequence (.seq)
- substructure atoms (.sca)
- model (.pdb)
- map coefficients (.mtz)
- map (.ccp4, .mrc, .xplor)
- NCS (.ncs)

The files from all of these formats will be converted to scalefactor (.sf), .seq, .sca(.sf), .pdb (.sf/model), .ncs.

If you have multiple data files from a single dataset, or if you have original data files with multiple observations, you can combine them into a single file using phenix.reflection_file_converter and then use the resulting file as the input to Autosol.

Additionally, within Autosol if you supply of substructure (unmerged original intensities or of ccp4 unmerged files or of .sca files) and a model, Autosol will combine the data from the substructure with the data from the model and write out a combined file. This combined file will be used in the rest of the Autosol run. Combining the data from the substructure and the model will allow Autosol to use information from the model in the initial scaling of the substructure information, or in other cases Autosol will use information from the model in scaling, so long as the model is in the same unit cell and has the same space group as the substructure information.

Sequence file format

The sequences for the current (and subsets) in the new letter code sequence of each chain in the structure to be solved. Sequences can be in any standard format (PIR, Fasta, plain text, etc). Sequences can be in one letter code or three letter code.

Example of a sequence file:

```
>1ubq:A:Ubiquitin-C52S, Ubc9 fusion protein
>1ubq:B:Ubiquitin-C52S, Ubc9 fusion protein
MQIFVKTLTGKTITLEVEPSDTIENVKAKIQDKEGIPPDQQRLIFAGKQLEDGRTLSDYNIQKESTLHLVLRLRGGMQIFVKTLTGKTITLEVEPSDTIENVKAKIQDKEGIPPDQQRLIFAGKQLEDGRTLSDYNIQKESTLHLVLRLRGGM
```

Usually the first line (after DNA, DNA, RNA,RNA) is a comment line. You can also specify it directly with a command such as mean_type=RNA.

Sequences can be in one letter code. They can be put on a single line and it will be used for all of them or they can be put on a separate line for each chain. Sequences can be in three letter code. If they are in three letter code they must be separated by a space. Sequences can be in any case, and be put in any set spaces, tabs, or tabs.

If there are more than one chain in the structure, then Autosol will use the sequence for the one that is the longest, and ignore the shorter sequences. Sequences can be entered in any standard fashion.

NOTE 1: Characters such as numbers and non-printing characters in the sequence file are ignored.

NOTE 2: Sequences can be in any case (upper or lower) and it will be read in the correct way. Blanks are ignored.

Datasets and Solutions in Autosol

Autosol keeps track of the data in a structure called an Dataset, which contains what is stored in a set of that data (for example, a set of Fobs and SIGFobs, or a set of Fplus, SIGFplus, Fminus, and SIGFminus). Autosol also keeps a structure called an Solution which contains information about the current solution (substructure, R-factors, CC, etc). Autosol also keeps a structure called an Solution which contains information about the current solution (substructure, R-factors, CC, etc). Autosol also keeps a structure called an Solution which contains information about the current solution (substructure, R-factors, CC, etc).

The Autosol wizard uses a "Selector" object to keep track of heavy-atom locations and the selected datasets that are used in the current solution. The Selector object also keeps a list of the current solutions and the current Dataset. Most of the commands in Autosol (including Phaser, Hyss, Resolve, Refmac, Phenix.refine, Phenix.refine, Phenix.hyss, Phenix.xtriage, Phenix.ccp4check, Phenix.xtriage, Phenix.ccp4check, Phenix.xtriage, Phenix.ccp4check

SIR dataset

We simulated data in a SIR dataset with the nature and derivatives, the sequence R_0, the heavy-short-tail, and the heavy-long-tail infection rate functions, and the sequence of the sum of the pairwise differences. Then we combined the six sim

```
$ ls -lh data/sir/sim-*.zarr.tar.xz data/sir/sim-*.zarr
-rw-rw-r-- 1 ubuntu ubuntu 1.1G Jun 15 00:00 data/sir/sim-deriv.zarr.tar.xz
-rw-rw-r-- 1 ubuntu ubuntu 1.1G Jun 15 00:00 data/sir/sim-R0.zarr.tar.xz
-rw-rw-r-- 1 ubuntu ubuntu 1.1G Jun 15 00:00 data/sir/sim-hst.zarr.tar.xz
-rw-rw-r-- 1 ubuntu ubuntu 1.1G Jun 15 00:00 data/sir/sim-hlt.zarr.tar.xz
-rw-rw-r-- 1 ubuntu ubuntu 1.1G Jun 15 00:00 data/sir/sim-spd.zarr.tar.xz
-rw-rw-r-- 1 ubuntu ubuntu 1.1G Jun 15 00:00 data/sir/sim-ssd.zarr.tar.xz
data/sir/sim-deriv.zarr:
total 12K
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zarr
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zgroup
-rw-rw-r-- 1 ubuntu ubuntu 1K Jun 15 00:00 .zmetadata
data/sir/sim-R0.zarr:
total 12K
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zarr
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zgroup
-rw-rw-r-- 1 ubuntu ubuntu 1K Jun 15 00:00 .zmetadata
data/sir/sim-hst.zarr:
total 12K
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zarr
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zgroup
-rw-rw-r-- 1 ubuntu ubuntu 1K Jun 15 00:00 .zmetadata
data/sir/sim-hlt.zarr:
total 12K
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zarr
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zgroup
-rw-rw-r-- 1 ubuntu ubuntu 1K Jun 15 00:00 .zmetadata
data/sir/sim-spd.zarr:
total 12K
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zarr
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zgroup
-rw-rw-r-- 1 ubuntu ubuntu 1K Jun 15 00:00 .zmetadata
data/sir/sim-ssd.zarr:
total 12K
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zarr
drwxrwxr-x 2 ubuntu ubuntu 4K Jun 15 00:00 .zgroup
-rw-rw-r-- 1 ubuntu ubuntu 1K Jun 15 00:00 .zmetadata
```

SAD with more than one anomalously scattering atom

We will add the dataset needed to use the new feature that accommodates anomalous scattering atoms. Note that data in the usual sims. Then specify any additional sims in the SIR dataset in the order of the IDs if you are running Kubinet with the command:

```
$ ./kubinet.sh sim-hst
```

Generally, you can add 1 sims and 1 dataset series values for the additional atom types with commands like:

```
$ ./kubinet.sh sim-hst sim-hlt sim-spd sim-ssd
$ ./kubinet.sh -d data/sir/sim-deriv.zarr.tar.xz -d data/sir/sim-R0.zarr.tar.xz -d data/sir/sim-hst.zarr.tar.xz -d data/sir/sim-hlt.zarr.tar.xz -d data/sir/sim-spd.zarr.tar.xz -d data/sir/sim-ssd.zarr.tar.xz
```

Note that the dataset series values for the additional atom types are not used in the current version of the model. Since it is unclear how to incorporate the information from the additional atom types, we will start by using only the data from the first atom type.

Now if you are running SAD on PRODID and your anomalously scattering atom is Sulfur, you will need to supply 1 set of anomalous scattering factors. If you are running SAD on a mixture of Sulfur and Selenium, you will need to supply 2 sets of f' and f'' values, one for each atom type.

A particularly useful way to use the Kubinet is to add 1 sims to a random structure that has SAD diffraction spots. Then, you can use the SAD phasing module in Phenix to see if it can find the sites of the anomalous scatterers and to solve the phase and so on. The sims dataset will be at /sim/sim.

MIR dataset

We will add the dataset from the SIR2 sims plus 1 simulation for the 2nd isomorph? Which you then run with Phenix phenix.find_ncs_from_ca and phenix.autosol with:

```
$ ./kubinet.sh -d data/sir/sim-deriv.zarr.tar.xz -d data/sir/sim-R0.zarr.tar.xz -d data/sir/sim-hst.zarr.tar.xz -d data/sir/sim-hlt.zarr.tar.xz -d data/sir/sim-spd.zarr.tar.xz -d data/sir/sim-ssd.zarr.tar.xz sim-hst
```

The MIR and SAD datasets will be stored separately from all Kinetic sims so that Kinetic will use differences or differences of differences between the MIR and SAD datasets. Note that the MIR and SAD datasets will be stored in /kinetic/sim/ subdirectory and the Kinetic phases will be stored in /kinetic/phase/.

Autofail with an extremely weak signal

We can set Kinetic sims with a very weak signal to autofail. The flag challenge is the kind of situation we want to avoid in the real world, so we want to be able to test how Kinetic handles it. Kinetic should fail on the following scenarios, including picking model with serious reasonable scores for the sites and long other scenarios. Kinetic should fail on the following scenarios, including picking model with serious reasonable scores for the sites and long other scenarios. Kinetic should fail on the following scenarios, including picking model with serious reasonable scores for the sites and long other scenarios.

```
$ ./kubinet.sh -d data/sir/sim-deriv.zarr.tar.xz -d data/sir/sim-R0.zarr.tar.xz -d data/sir/sim-hst.zarr.tar.xz -d data/sir/sim-hlt.zarr.tar.xz -d data/sir/sim-spd.zarr.tar.xz -d data/sir/sim-ssd.zarr.tar.xz sim-hst
```

For the weakly modified sims, there is a keyword /autoinc, and that may be helpful in cases where the /autofail keyword is not sufficient.

```
$ ./kubinet.sh -d /sim
```

The keyword works with the keyword /fail. For /autoinc, it is determine whether a set of detectors for density modification and phasing is sufficient to solve the structure. If the /autoinc keyword is used, Kinetic will use the /DM flag to select the detectors and density modification. /autoinc and /fail can be used in the same command.

Autofail with a cluster compound

The sim will be generally a random and a cluster compound that PDB or PDBC with. Normally you should supply a PDB file with an example of the codes with the keyword /pdb, with the cluster compound and a unique identifier. Kinetic will use the cluster compound to make the sites and phase the sim. If the /pdb keyword is not used, Kinetic will use a random cluster. Cluster compounds can be used in the same command as /fail and /autoinc.

R-free flags and test set

R-free flags are used to keep the test set. Kinetic will use the test set that is in the file. Normally Phenix sets up the test set. Kinetic uses a 5 Å cutoff. In the PDB set, the R-free percentage is always at 5 through 10 with 5 as the most common. Kinetic should be able to handle any R-free flag set up by Phenix. Kinetic should be able to handle the R-free flag set up by the Kubinet module should fit in the R-free set up by Kinetic.

Specific Simulations and problems

- The use of the parameters and the Kinetic/Kubinet/PDBC/PDBC of the Kubinet system is limited by the parameters and the Kinetic/Kubinet/PDBC/PDBC of the Kubinet system. Kinetic/Kubinet/PDBC/PDBC/PDBC

```
# Experimental phasing in the AutoSol GUI
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* Introduction
* Video Tutorial
* Input data and mandatory parameters
* Running AutoSol
  * Output files
  * Heavy-atom search
  * Phasing and density modification
  * Model-building
  * What to do if AutoSol fails
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  * Wizards for X-ray data
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## Introduction

AutoSol is provided mainly as a means to demonstrate for users and pro-ver-tender (and AutoSol-in-development) developers that there are a comprehensive collection of tools for phasing macromolecules in the phenix distribution. Here is a brief overview of some of the range of options and functionalities.

The AutoSol wizard provides a simple interface to automatically run a standard macromolecular phasing workflow. This wizard is ideal for structure crystallographers who are not experts in macromolecular phasing and who want to try a standard set of options and see what happens. The wizard also provides a convenient interface for those who are experts in macromolecular phasing and who want to try a variety of options and see what happens.

The AutoSol wizard can be used for a variety of phasing methods, including multiple wavelength anomalous dispersion (MAD), single wavelength anomalous dispersion (SAD), multiple isomorphous replacement (MIR), multiple isomorphous replacement with anomalous scattering (MIRAS), and molecular replacement (MR). The wizard can be used for phasing from scattering from any one of a variety of scatterers, including selenium, sulfur, heavy atoms, and anomalous scatterers. The wizard can be used for phasing from data from a variety of sources, including synchrotron, home source, and electron diffraction. The wizard can be used for phasing from data from a variety of crystal forms, including protein, DNA, RNA, and small molecule crystals. The wizard can be used for phasing from data from a variety of resolutions, including low resolution (3 Å and lower), medium resolution (3 Å to 1.5 Å), and high resolution (1.5 Å and higher).
```

build_one_model

Phenis

Phylo-Linguistic Bioinformatics Environment for Integrated Multiparadigm Analysis

Quick model building of a single model with resolve using build_one_model

Author(s)

- Tanel_one_header Tanel Kaasalaagi

Purpose

If you have an one .nwk newick tree file and a sequence file, you can use build_one_model to just build a single model with resolve. You can also combine all splitting models.

Usage

How build_one_model works:

Build_one_model uses iqtree2 standalone binary to build a single model in supplied .nwk newick. If you supply a model, then iqtree2 will use that model. Otherwise iqtree2 will use default model.

Output files from build_one_model

build_one_model.sh - A file that calls the iqtree2 binary

Examples

Standard run of build_one_model:

Running build_one_model is easy. From the command line you can type:

```
./build_one_model.sh -tree tanel.nwk
./build_one_model.sh -tree tanel.nwk -seq tanel.fasta
```

where tanel.tree, phylo_tanel.fasta files can your file & fasta for refinement. If you want to supply a FEB file you can add it with -feb option:

```
./build_one_model.sh -tree tanel.nwk -seq
./build_one_model.sh -tree tanel.nwk -seq phylo_tanel.fasta -feb tanel.feb
```

Possible Problems

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
header_tanel
    -tree <file>                    Tree file
    -seq <file>                     Alignment file
    -dna|-aa|-mix|-codon            Sequence type
    -feb|-ratio|-rate|-mrate        Input FEB file
    -model <model_name>             Substitution model
    -fast|-mem|-safe|-lmem          Speed/memory/safe mode
    -nt|-nt2|-nt3                   Nucleotide codon position
    -mrate <rate_list>              Rate multipliers
    -mfreq <freq_list>              Mixture frequencies
    -mtree <file_list>              Multi-tree file
    -mdef <file_list>               Mixture definition file
    -mdtree <file_list>             Multi-tree mixture definition
    -mdef+ <mixture_def>            Inline mixture definition
    -mdef+tree <mixture_def_tree>   Inline mixture definition with tree
    -mdef+freq <mixture_def_freq>   Inline mixture definition with freq
    -mdef+rate <mixture_def_rate>   Inline mixture definition with rate
    -mdef+mrate <mixture_def_mrate> Inline mixture definition with mrate
    -mdef+model <mixture_def_model> Inline mixture definition with model
    -mdef+feb <mixture_def_feb>     Inline mixture definition with FEB
    -mdef+mfreq <mixture_def_mfreq> Inline mixture definition with mfreq
    -mdef+mdtree <mixture_def_mdtree> Inline mixture definition with mdtree
    -mdef+mdef <mixture_def_mdef>   Inline mixture definition with mdef
    -mdef+dna|-aa|-mix|-codon       Inline mixture definition with seq type
    -mdef+nt|-nt2|-nt3              Inline mixture definition with codon position
    -mdef+fast|-mem|-safe|-lmem     Inline mixture definition with speed/memory/safe
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    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+model <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_model> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and model
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+feb <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_feb> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and FEB
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mfreq <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mfreq> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and mfreq
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdtree <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdtree> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and mdtree
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and mdef
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+ <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef+> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+dna|-aa|-mix|-codon Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and seq type
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+nt|-nt2|-nt3 Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and codon position
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+fast|-mem|-safe|-lmem Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and speed/memory/safe
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+model <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_model> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and model
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+feb <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_feb> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and FEB
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mfreq <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mfreq> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and mfreq
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdtree <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdtree> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and mdtree
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef <mixture_def_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef_mdef> Inline mixture definition with inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and inline mixture definition and mdef
    -mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef+mdef
```

cobham_training

Phenix *Python based Hierarchical ENvironment for Integrated Xtallography*

Structure Exploration with CeBLAM Training

Authors

Jeremy Jeanson, Christopher Williams (Richardson Lab, Duke University)

Purpose

CeBLAM training is provided as part of workshop tools for analyzing cryo-EM and other crystallographic or cryoEM structures. This training provides a brief introduction to the CeBLAM tools and interfaces, and to the Phenix GUI. It includes a brief introduction to the Phenix GUI, and to the Phenix Model Manager, which provides a convenient way to manage resources and output structures. Most of the training uses the amazing toolset and amazing information-rich interface of the Molprobity/Phenix Ramachandran Plot, which provides a wealth of information about structures.

For information on cobham_training, the main user-end interface for CeBLAM, please refer to the documentation for cobham_training.

The Short Version

Run cobham_training and the following help=True or the commandline will provide fairly complete documentation. The help menu is intended to augment or add supplement that documentation, not replace it.

How CeBLAM Training Works

The cobham_training tool provides a convenient way to run a training calculate general geometry measures selected by the user. It will run all these measures on the current selected selections. These selections may be residues or if the selection is a chain, the selection will be interpreted as a structure-level or chain-level.

Available Measures

Many standard measures are available through cobham_training. These include: - Lower Five Ramachandran Diheds: Lowerer five the expected Ramachandran Diheds, that is psi 2 and phi-1 in addition to phi and psi. - Cbeta Dev: Cbeta deviation - Omega: Omega the peptide bond dihedral (used to define 3 in cbeta dev)

CeBLAM measures

CeBLAM provides a number of structurally meaningful measures of protein geometry. - Two CA-defined pseudo-dihedrals, the CA0D2 (CD2 in other sw) or 2-defined by the CA atoms of 2 residues and the 3 that are two-out-of-three residues in the 4-residue sliding window. - Two CA-defined pseudo-angles, the CA0A2 (CA2 in other sw) and CA1A2 (CA3 in other sw) - Two CA-defined pseudo-bond lengths, the CA0D2 (CD2 in other sw) and CA1D2 (CD3 in other sw) - Two CA-defined pseudo-dihedrals, the CA0D2 (CD2 in other sw) and CA1D2 (CD3 in other sw)

Action-based Structural Measures for Enhanced Rationality

CABLAM Validation in Phenix

Authors

Lizbeth, Jackson, Christopher Williams (Richardson Lab, Duke University)

Purpose

CABLAM stands for C-Alpha Based Low-resolution Annotation Method. It is a system designed to use protein CA geometry to predict and validate protein structures. It is particularly well suited to cryo-EM data, but it can also be beneficial for use in low resolution structure where occupancy of some of residues or a loop can cause the rest of the structure to look worse than it is, or for homologous or similar structures, where it can be informative of differences.

How CABLAM works

For each residue, cablam_validate calculates several measures based on CA geometry. It uses these measures to identify outliers, and to predict the most likely correct conformation for outlier residues. Outlier identification is based on a combination of the measures, and is described in the cablam_validate section of the manual and in Lizbeth's dissertation.

Lizbeth: cablam_validate compares local CA geometry measures which are robust at low resolution against contours of those measures observed in high resolution structures. Outliers are flagged when observed measurements are found to be unlikely enough to be worth a second look.

Running CABLAM Validation

Lizbeth: Run cablam_validate.py on a PDB file corresponding to a single C-alpha trace, or a structure file that phenix.find_ca.models recognizes.

phenix.cablam_validate file.pdb output.cablam.pkl -out_txt.obj -no_pkl -overlap -text -points

Outlier Cutoff

Lizbeth: The default cutoff is 0.5 for cablam. This cutoff is for flagging of modeling errors, but also may inadvertently flag outliers and local conformations such as kinks in loops.

-cutoff=0.1 will be more conservative but still catch most outliers.

-cutoff=0.01 will be recommended for use with output to phi.

Numerical output modes are available

Full Run

Lizbeth: At, or close to, most comprehensive validation output, recommended for general use. If geometries are automatically refined flag in the working directory. This cablam_test.txt and the cablam_test.pkl, then opens the output files and prints a summary of the results. This summary includes the number of residues of each type, and a CSV-formatted section for CA geometry outliers. This can be cut-and-pasted into a spreadsheet program for further analysis. This can be helpful for comparing the effect of different cutoffs, or for comparing a model before and after refinement. The -text option suppresses the CSV section, and prints only the human-readable, fixed-width, tabular output.

CA Kin

Lizbeth: At, or close, cutoff=0.1PDB similar to backrub timeseries for C-Alpha geometry to screen. This markup output is intended to be a prototype of the backrub timeseries for C-Alpha chemical kinematics generated by phenix.ksharpen. CABLAM is dependent on CA geometry, so it is necessary to know where that geometry is unusual. This markup output is intended to be a starting point for a tool to flag, for example, CA-only models for manual review, or to highlight regions of a cryo-EM reconstruction that look like backbone but don't fit the sequence. Note that the outlier_cutoff must be set very low for this output, or most residues will be flagged.

Oneline

-oneline prints a single line summary of CABLAM statistics for each of the submitted proteins. Sample output follows:

```
phenix.cablam_validate -oneline pdb_test_parser_pdb.pdb,pdb_test_parser_cif.cif,pdb_test_parser_pdb.ent
pdb_test_parser_pdb.pdb
```

- **pdbid** identifies the input file
- **residues** gives the number of interpretable residues assessed by CABLAM (residues near termini and chain breaks are not interpretable by CABLAM)
- **outliers** gives the number of CA geometry outliers, and **outlier_percent** gives the percent of residues that are outliers
- **contours_percent** gives the percent of residues with "unusual" outlier scores (higher than 0.5), by the default cutoff
- **rotatoins_percent** gives the percent of residues with "unusual" rotamer scores (higher than 0.5), by the default cutoff
- **cablam_score** gives the percent of residues with CA geometry outliers, higher than 0.5% may be cause for concern

Text

-text is the default. This provides concentrated, comma-separated records for each outlier residue. Sample output follows:

```
CA: 0 -> 10:A:1:GLY:0.0000:0.0000:0.0000:0.0000
CA: 0 -> 10:A:2:ARG:0.0000:0.0000:0.0000:0.0000
CA: 0 -> 10:A:3:ARG:0.0000:0.0000:0.0000:0.0000
CA: 0 -> 10:A:4:ARG:0.0000:0.0000:0.0000:0.0000
CA: 0 -> 10:A:5:ARG:0.0000:0.0000:0.0000:0.0000
```

- **residue:** A list residue identifier for the outlier
- **contour_score:** A CA geometry based measure of which the residue falls in Fraction form (lower of 2 scores, when taking a score above cutoff 0.5% of the default cutoff for cutoff=0.1)
- **bump_score/rotamer_score:** Same as for contour_score, but for the separate score that looks only at the rotamer outlier and bump outlier measures, respectively. Not used for cutoff selection, but may be informative for manual review.
- **forward_bump/backward_bump:** Forward flags for unusual bump distances, higher means unusual spacing. Backward flags for unusual bump distances, higher means unusual spacing. Not used for cutoff selection, but may be helpful for manual review.
- **cablam_score:** A CA geometry based three-box score between 0 and 1, higher values indicate greater confidence that the residue should be modeled as three-box kink. Not default cutoff in 0.5pre

Points

-points prints points to screen in BASH of points in kinemage format to produce a pointcloud of outlier residues in CABLAM space. Primarily a developer tool.

Records

-records allows records to screen JSON and DIMPLE-type records for secondary structure elements identified by CABLAM. Formatting for these records is not yet totally consistent with PDB standards, but will be brought into closer alignment soon.

Lizbeth: Records are not currently available through the phenix.cablam_find, but will be available on a future version of the cablam.py

Tools for exploring lower structures are available through cablam_tutorial

carbo_primer

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

Carbohydrate Primer

Introduction

A carbohydrate is an organic compound with the empirical formula $C_m(H_2O)_n$(where m could be different from n). Carbohydrates are the most abundant biomolecules that differentiate them. These include

- abundance of chiral centers
- ring-chain tautomerism
- existence of cyclic acetals
- existence of glycosidic bonds
- linear or cyclic

Linear carbohydrates are named as aldo or keto isomers based on the position of the OX on the anomeric carbon relative to the axial group of the ring.

Protein Chemistry

If your protein was produced in or raised in yeast cell line, you should only have N/O-linked sugars. Mammalian cell lines can add a lot of types of PTM like O-ser which the the density better if you know any details about the sugar, the sugar units?

MAN

Mannose is a common epimerate in protein chemistry. There are two linear isomers and two cyclic forms of mannose. The cyclic form can exist in different isomeric forms of the different anomeric equals to axial. A leading form of alpha is axial-axial and subsequently is the one of the three linear isomer. Thus, alpha is the leading form of mannose in solution and the majority of cyclic form is the alpha form of mannose in DPB.

D-MANNOSE

D-MANNOSE

D-ALDO-D-MANNOSE

D-KETO-D-MANNOSE

NAG

NAG represents the beta form (the most common) and NGS is the alpha form. NAG is interesting because it's a decorated sugar. It is attached to the N of Asn.

D-GLUCOSE-N-ACETYLAMINE

1,3-BETA-GRIDO-1,6DIACETOPRANOSE

D-GLUCOSAMINE,1,6-DIACETOPRANOSE

Polysaccharides

Polysaccharides are long chain molecules that consistsly linet to proteins. The links between are generally between the anomeric carbon and an oxygen of the "consecutive" units moving from the protein outward on the chain. Below is a typical N-linked glycan structure.

Note that the left spectrumb is linked with the anomeric carbon sep an oxygen to the C3 carbon. The left unit is D-mannose and the right unit is galactose. The link is known as 1-3 or disaccharide "sequence" and is a and link is beta-D-Gal.

Protein links

The main common link to proteins is the n link which attaches to ASN in the ASN-X-SER/THR motif.

Phenis — Python Issues Resolved Enhanced for Integrated Mathematics

Comparison of CA positions to two models allowing any order of fragments

Author(s):

- J. Joel Jeremiah Tom Tarawneh

Purpose

Identify how many of the CA atoms in one model match CA atoms in another model. Separately identify how many of the CA atoms in the target structure are the mates of the model atoms.

Usage

How chain_comparison works:

chain_comparison now normally selects the chains and of the target model (the first model specified), then it selects the chains and of the model (the second model specified). Then it selects the CA atoms in the residues in the specified range. If NCS is requested, the unique part of the specified NCS is selected, NCS is applied and this the atoms in the specified range.

If desired, you can make chain_comparison write out all the atoms in the specified chains that are matching and not matching in the target model.

Examples

Standard use of chain_comparison:

Running chain_comparison is easy: from the command line you can type:

```
phenix.chain_comparison model.pdb model.pdb
```

If you want to compare 2 positions for RMSD/NN/ref, you can see:

```
phenix.chain_comparison model.pdb model.pdb rmsd=yes
```

Possible Problems

Specific limitations and problems:

Literature

Additional information:

List of all available keywords:

```
model PDB
  pdb_in = None                  Input PDB file
  pdb_out = None                 Output PDB file
  chain_match_pdb = True         Use chain match (chain id) when matching pdb_in and
                                 pdb_out
  chain_match_pdb_in = True      Use chain match (chain id) when matching pdb_in and
                                 pdb_out
  chain_match_pdb_out = None     Force pdb_out chain to match pdb_out chain pdb_out=c
  rmsd = False                   Calculate RMSD
  rmsd_part_of_target_pdb = False  If True model pdb_in is part of the target pdb model
                                 (pdb_out) and the rest of the target pdb model
                                 (pdb_out) is ignored.
  write_selections = False       Write out selections to a file and exit. Default: not
                                 write selections
  chain_filter = None            Only consider chains in this list (for example
                                 chain=A chain=B)
                                 Note: this is different from chain_match_pdb which
                                 is used to select matching chains. This keyword
                                 allows you to specify which chains to use in
                                 comparison. Default: all chains are used
                                 Note: if chain_filter is specified and chain_match_pdb
                                 is True, chain_filter is used to select chains from
                                 both models. If chain_filter is not used, the chains
                                 from the first model are used to select chains from
                                 both pdb_in and pdb_out.
  write_matching = False         Write out matching atoms to pdb_out and exit. Default:
                                 not write out matching atoms
  only_ca = False                Only use CA atoms in comparison (default: use all
                                 atoms in specified residues)
                                 Note: if only_ca is True, only CA atoms are used in
                                 comparison, regardless of other keywords such as
                                 ignore_hydrogens, ignore_ca, ignore_cb, ignore_mainchain
                                 and ignore_sidechain.
  ignore_ca = False              Ignore CA atoms in comparison (default: use all atoms
                                 in specified residues)
  ignore_cb = False              Ignore CB atoms in comparison (default: use all atoms
                                 in specified residues)
  ignore_mainchain = False       Ignore mainchain atoms in comparison (default: use all
                                 atoms in specified residues)
  ignore_sidechain = False       Ignore sidechain atoms in comparison (default: use all
                                 atoms in specified residues)
  ignore_hydrogens = True        Ignore hydrogen atoms in comparison (default: use all
                                 atoms in specified residues)
  ignore_ca_not_in_target = True Ignore CA atoms in pdb_in that are not in the target
                                 pdb model (pdb_out)
  ignore_ca_not_in_model = False Ignore CA atoms in the target pdb model (pdb_out)
                                 that are not in the model pdb_in
  ignore_ca_not_in_both = False  Ignore CA atoms in pdb_in that are not in the target
                                 pdb model (pdb_out) and CA atoms in the target pdb
                                 model (pdb_out) that are not in the model pdb_in
  ignore_ca_not_in_both_in_pdb_in = False  Ignore CA atoms in pdb_in that are not in
                                 the target pdb model (pdb_out) and CA atoms in the
                                 target pdb model (pdb_out) that are not in the model
                                 pdb_in
  ignore_ca_not_in_both_in_pdb_out = False  Ignore CA atoms in the target pdb model
                                 (pdb_out) that are not in the model pdb_in and CA
                                 atoms in pdb_in that are not in the target pdb model
                                 (pdb_out)
  remove_ca_not = False          Remove CA atoms that are not in the target pdb model
                                 (pdb_out)
  keep_group = None              Keep only atoms in the specified group
  write_by_keep_group = False    Write out atoms by keep_group
  write_keep_keep_other = False  Write out keep_group and other atoms
  ncs_pdb = None                 Use these NCS operations when writing out pdb_out
  ncs
    ncs_file = None              NCS file
    ncs_text = None              NCS text
    ncs_type = None              Type of NCS (rotation, translation, or
                                 rotation-translation)
    ncs_number = None            Number of NCS operations to apply
    ncs_center = None            Center of NCS rotations (x,y,z)
    ncs_rms = None               RMS of NCS operations
    ncs_group_number = None      Group number to use from NCS file
    ncs_chain_suffixes = None    Chain suffixes to use for NCS ops (for example
                                 A,B,C,D)
    ncs_omit_selection = None    Omit this selection when applying NCS
    ncs_coordinate_system = None Coordinate system (PDB, Cartesian, or Fractional)
    ncs_write_ncs_info = False   Write out NCS information
    ncs_apply_to_all_chains = False  Apply NCS to all chains in PDB file
    ncs_write_ncs_to_pdb = False Write out NCS to PDB file
  output
    verbose = False              Verbose output
    quiet = False                Quiet output
    debug = False                Debug output
    output_dir = None            Output directory
    output_prefix = None         Output prefix
    output_suffix = None         Output suffix
    overwrite = False            Overwrite existing files
    scientific = None            Use scientific notation for output
    precision = 3                Number of digits after decimal point
    wide = False                 Do not wrap output to 79 characters
    comments = True              Include comments in output files
    comment_character = None     Character to use for comments in output files
    prefix_with_comment_character = False  Prefix output with comment character
    remark_number = None         Remark number to use for output
    remark_text = None           Remark text to use for output
    remark_prefix = None         Prefix for remark lines
    remark_suffix = None         Suffix for remark lines
    log = None                   Log file
    log_append = False           Append to log file
    log_to_stdout = True         Write log to stdout
    log_to_stderr = False        Write log to stderr
    log_buffer = False           Buffer log output
    log_buffer_lines = None      Number of lines to buffer
    log_buffer_bytes = None      Number of bytes to buffer
    log_buffer_flush_level = None  Level at which to flush buffer
    log_buffer_flush_to_disk_on_exit = False  Flush buffer to disk on exit
    log_buffer_flush_to_disk_on_warning = False  Flush buffer to disk on warning
    log_buffer_flush_to_disk_on_error = False  Flush buffer to disk on error
    log_buffer_flush_to_disk_on_critical = False  Flush buffer to disk on critical
    log_buffer_flush_to_disk_on_exception = False  Flush buffer to disk on exception
    log_buffer_flush_to_disk_on_interval = None  Flush buffer to disk on interval
    log_buffer_flush_to_disk_on_size = None  Flush buffer to disk on size
    log_buffer_flush_to_disk_on_percent = None  Flush buffer to disk on percent
    log_buffer_flush_to_disk_on_memory = None  Flush buffer to disk on memory
    log_buffer_flush_to_disk_on_time = None  Flush buffer to disk on time
    log_buffer_flush_to_disk_on_custom = None  Flush buffer to disk on custom condition
    log_buffer_flush_to_disk_on_custom_function = None  Flush buffer to disk on custom function
    log_buffer_flush_to_disk_on_custom_function_arguments = None  Arguments for custom function
    log_buffer_flush_to_disk_on_custom_function_kwargs = None  Keyword arguments for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value = None  Return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type = None  Type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_name = None  Name of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module = None  Module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_name = None  Name of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version = None  Version of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number = None  Version number of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_major = None  Major version number of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_minor = None  Minor version number of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_patch = None  Patch version number of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build = None  Build version number of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_pre_release = None  Pre-release version number of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_post_release = None  Post-release version number of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_dev = None  Dev version number of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_local = None  Local version number of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata = None  Build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash = None  Hash of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm = None  Hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_name = None  Name of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version = None  Version of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number = None  Version number of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_major = None  Major version number of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_minor = None  Minor version number of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_patch = None  Patch version number of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build = None  Build version number of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_pre_release = None  Pre-release version number of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_post_release = None  Post-release version number of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_dev = None  Dev version number of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_local = None  Local version number of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata = None  Build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash = None  Hash of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm = None  Hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_name = None  Name of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version = None  Version of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number = None  Version number of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_major = None  Major version number of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_minor = None  Minor version number of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_patch = None  Patch version number of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build = None  Build version number of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_pre_release = None  Pre-release version number of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_post_release = None  Post-release version number of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_dev = None  Dev version number of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_local = None  Local version number of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata = None  Build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash = None  Hash of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm = None  Hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_name = None  Name of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version = None  Version of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number = None  Version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_major = None  Major version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_minor = None  Minor version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_patch = None  Patch version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build = None  Build version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_pre_release = None  Pre-release version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_post_release = None  Post-release version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_dev = None  Dev version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_local = None  Local version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata = None  Build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash = None  Hash of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm = None  Hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_name = None  Name of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version = None  Version of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number = None  Version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_major = None  Major version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_minor = None  Minor version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_patch = None  Patch version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build = None  Build version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_pre_release = None  Pre-release version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_post_release = None  Post-release version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_dev = None  Dev version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_local = None  Local version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata = None  Build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash = None  Hash of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm = None  Hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_name = None  Name of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version = None  Version of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number = None  Version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_major = None  Major version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_minor = None  Minor version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_patch = None  Patch version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build = None  Build version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_pre_release = None  Pre-release version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_post_release = None  Post-release version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_dev = None  Dev version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_local = None  Local version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata = None  Build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash = None  Hash of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm = None  Hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version = None  Version of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number = None  Version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_major = None  Major version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_minor = None  Minor version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_patch = None  Patch version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build = None  Build version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of module of type of return value for custom function
    log_buffer_flush_to_disk_on_custom_function_return_value_type_module_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_build_metadata_hash_algorithm_version_number_pre_release = None  Pre-release version number of hash algorithm of build metadata of hash algorithm of build metadata of hash algorithm of build metadata of hash
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chatbot

Python based Hierarchical Phenotyper for Extended Ontology

Using the Phenix chatbot assistant

Authors

+ Ingo Hindrichs, Peter Grant, Thomas C Terwilliger

Purpose

The Phenix chatbot is intended to guide Phenix users through the steps in structure determination, to provide information about the Phenix software, to answer questions regarding topics in the cryo-EM biological predictions SIG or in the Phenix discussion forum.

How the chatbot works

The Phenix chatbot is based on Google Bard/Gemini. The chatbot was supplied with over 200 pages of Phenix documentation, all the Phenix tutorialtexts, most of the Phenix video tutorials, and some of the Phenix discussions.

The chatbot can be started with this link. You have to log into a Google account (any Google account should work) and then you can start asking questions.

The chatbot has a Google-styled chatbot interface consisting mainly of a textbox that it will use, a text window where you type in questions and the chatbot answers, and a Google-styled text window to open controls.

Initially, you will see the Chat section. You can ask any questions about how to use Phenix and how to interpret results.

In the Media section, you can listen to an audio summary (a podcast) of structure determination with Phenix. Clicking on the Tutorials section will provide a list of tutorials that the chatbot can suggest to you, and clicking on a tutorial will start it.

Clicking on the Discussions section opens to the Chat section. A left pane appears after its opening. When you click on a topic, it opens up a query in the Google search and highlights text at the point where it will be found in the chat. If the search is a dead end, you can scroll to the top of the search and hit the pencil icon to edit the query.

What kind of questions you can ask the chatbot

The chatbot has limited phase-solving, but the primary purpose is dealing with questions like:

```
"How do I solve my structure?"
"What is the difference between phenix and xtal?"
"Can I search a model for ensembles?"
"How do I run refinement?"
"Phenix.refine gives me an error saying that part of the matrix
 is not positive definite. What do I do?"
"Please tell me how to run molecular or ab initio replacement"
"How do I run phenix.ccp4mr?"
"How do I tell if I have a good model? Is an R-value of 0.35 ok?"
"What right phase or map coloring strategies do use?"
```

Limitations of the chatbot

The chatbot is limited to the sources that is supplied with, so it only knows about Phenix, and it only knows what Phenix documentation, tutorials, and discussions have been supplied to it.

It matches the text you ask and can make mistakes and give incorrect answers. This does not seem to happen much if the answers are simple, but you need to always be on alert when using it. Unlike the chatbots at a Major Tech company, it does not learn.

It does not remember the text you ask and the answers it gives from one session to another. It does remember the text you ask and the answers it gives in a session, but it does not apply reasoning if you are comparing a model one in a way because that was not asked in the documentation.

It does not know how to do anything with your data, it does not know how to do anything in a lab and never always looked at. For example, it does not know molecular replacement, molecular dynamics, NMR, and cryo-EM. It does not know how to do anything with your data but change the resolution in the reconstruction. It does improve the phase information.

Phenix *Active-based Prioritized Phenotypes for Extended Bibliography*

Using the Phenix chatbot assistant

Authors

- Pepe Ferrando, Peter Zoupe, Thomas C Terwilliger

Purpose

The Phenix chatbot is designed to guide Phenix users through the steps in structure determination, to provide answers to Phenix-related questions, to suggest debugging help (logs, a file with debugging problems, and so on) relevant for the Phenix software/forum.

How the chatbot works

The Phenix chatbot is based on Google Notebook/R. The notebook was supplied with over 600 pages of Phenix documentation, including the complete contents of the Phenix video tutorials, and copies of the Phenix bulletinboard.

The chatbot can be started with this page. You have to log into a Google account (any Google account should work). This creates a new clone copy of the notebook.

The notebook has a Sources section containing a list of materials that it will use, a Chat section where you type questions and see responses, and a Studio section where you can create various kinds of output.

Normally you will use the Chat section. You can ask any questions about how to use Phenix and how to interpret Phenix output.

In the Studio section, you can listen to an audio summary (a podcast) of structure determination with Phenix. You can create a "Briefing document" (below) and ask questions directly (and the tools will answer you in the middle of their output).

When the chatbot answers your questions in the Chat section, it will pull citations after its responses. When you click on the citations, the chatbot will show the exact sentences from the paper that it used to make its responses. If the source is a table, you can scroll to the top of the source and the complete table will be shown.

What kind of questions one can ask the chatbot

You can ask the chatbot almost anything. Here are some questions in details.

For example:

```
"What is using as structure?"

"Can I use chatbot with a new data?"

"What inputs do I need for polaris?"

"How to install chatbot?"

"How is input and output structure that you' ve extract and the machine-
ready of the active site residues in the paper?"

"How is the output structure of the paper chatbot?"

"How do I know if my molecule is active?"

"How do I tell if I have a good model? Is an R-value of 0.25 ok?"

"What paper created the Polaris AI structure by ML?"
```

Limitations of the chatbot

The chatbot only knows about the papers we supplied with, so it only knows about Pharos, and it only knows what it is told by the documents, the chatbot and modelling, and the papers we have supplied.

AI models like this can and can make mistakes and give incorrect answers. The data not seem to happen in the training data, and the model will try to fill in the gaps with what it thinks is most likely, which can be a good guess or a wild guess.

Because it always tries to be helpful and consistent, the chatbot will not know if, for example, the correct answer of the chatbot does not know that for the pharos map complexes but you could supply a molecular if you are knowledgeable about the pharos map complexes and the chatbot will accept it.

While the chatbot can give potentially correct overviews of how to solve a structure, sometimes it can get small details wrong, such as the exact number of the residue, or the exact sequence of the residues. This can may be true for crystallo density modification does not change the resolution in X-ray crystallography, it only improves the phase information.

PHENIX *Python-based Hierarchical Environment for Integrated Crystallography*

Importing structures from the PDB

Unlike most other reflection formats, the CIF files used by the PDB to store experimental data are not supported by the CCP4 libraries. Instead, we have written our own parser, which should be able to read any valid mmCIF structure file. Although the structure factor data are stored in a different format, the PDB does provide a subset of the mmCIF data in a format that is compatible with the CCP4 libraries, and we have written a separate parser for this.

Using the PHENIX GUI

Open the main GUI and click "Import of structure factors" under the "Reflections tool" category. Only the CIF structure factor files will be listed in the file chooser, and the output will be in CCP4 MTZ format. Unless you need to quickly take "pure" F (any extra PHENIX fix is a sanity check on the detailed amplitudes) which may not be appropriate:

If one loads the PDB 3l1wn format(s) downloaded for necessary files and, you can simply enter the 3l1 into the "Input file" field (enter and click "Run", and the PDB will be read and converted, then the MTZ will be saved.

Command-line use

The command-line program has the modified arguments to show below:

```
phenix.mtz2cif -h
usage: phenix.mtz2cif [options] [-f file] [keywords]

Options:
  -h, --help    show this help message and exit
  -f FILE, --file=FILE, --mtz=FILE
                Input CCP4 MTZ file (required)
  -o FILE, --output=FILE, --cif=FILE
                Output mmCIF file (default: stdout)
  -l LABELS, --labels=LABELS
                Comma-separated array labels
  -c CRYSTAL, --crystal=CRYSTAL
                Crystal name (default: first)
  -d DATASET, --dataset=DATASET
                Dataset name (default: first)
  -n NAME, --name=NAME
                Name of the data block (default: data_phenix)
  -p PREFIX, --prefix=PREFIX
                Prefix for output data block
  -s, --sigma, --sigmaf, --sigma_f, --sigmafsq, --sigma_fsq
                Output sigma or sigma-squared values
  -r, --rfree, --rfree_flag, --free, --free_flag, --free_r_flag
                Output R-free flag
  -a, --all     Output all data and array labels
  -v, --verbose, --debug
                Verbose output
  -q, --quiet   Suppress output
  --no-rfree    Do not output R-free flag
  --no-sigma    Do not output sigma values
  --no-ccp4     Do not output CCP4 data structure keywords (default: output)
  --no-cif      Do not output mmCIF data
  --keep-fc, --keep-calc, --keep-calculated
                Keep calculated structure factors (default: omit)
  --keep-fo, --keep-obs, --keep-observed
                Keep observed structure factors (default: omit)
  --keep-all    Keep all data (default: omit unknown and incomplete)
  --keep-ccp4   Keep CCP4 data structure keywords (default: omit)
  --keep-cif    Keep mmCIF data (default: omit)

usage: phenix.mtz2cif [options] [-f file] [-o output] [keywords]
```

The program will automatically determine which are the important arrays and keywords information, in these cases you should use the associated flag (for flags of the other options all values not necessarily full, just input a dummy flag or value, e.g. -f file -o output).

As a shortcut to download the files from the RCSB (or mirror) website, PHENIX includes a tool for fetching data. Simply type:

```
phenix.fetch_pdb 3l1w phenix.fetch_pdb -p 3l1w
```

The properties "-r" specifies that the structure factors should be downloaded instead of the PDB file. (This will only work if the structure deposited that data.)

Output

Assuming that the data were successfully extracted, the program will create an MTZ file with columns FOBS, SIGFOBS (they will be treated as proxies for true amplitudes in PHENIX) and R-free flags. In any cases there is a warning about the R-free flag being "not a valid R-free flag" (this is OK, this is the R-free flag, it just means that it is not in the standard CCP4 format). Also there is the CIF file, this is the ASCII version of the converted or otherwise unintelligible values.

citations

Phenix

Reflection Matrix Model Refinement for Crystallography

List of references related to Phenix

Current primary Phenix citation:

- **Macromolecular structure determination: comparison of crystallographic and electron microscopy methods in Phenix.** P. V. Afonine, T. C. Baranova, R. I. Sarni, R. D. Adams, P. H. Zwart, T. C. Terwilliger, A. Brunger, P. D. Adams, Acta Crystallogr. D Struct. Biol. 75, 1114 - 1124 (2019). doi:10.1107/S2059798319011471 Acta Crystallogr. D Struct. Biol. 75, 1114 - 1124 (2019). doi:10.1107/S2059798319011471

Other articles

The following articles have been produced by members of the Phenix collaboration, and mainly by selected developers of the Phenix software.

- **Accounting for nonuniformity of bulk solvent: a mosaic model.** P.V. Afonine, P.D. Adams, D.G. Waterman, Acta Crystallogr. D 75, 1 - 8 (2019).
- **Evaluation of X-ray crystallography powder neutron diffraction data.** M. Meyers, J. Hoyung, and P.V. Afonine, Acta Cryst. (2018).
- **Joint X-ray and neutron refinement with Phenix and CCTBX.** P.V. Afonine, M. Meyers, P.D. Adams, A. Brunger, Acta Crystallogr. D Struct. Biol. 74, 239 - 255 (2018). doi:10.1107/S2059798318002425 Acta Crystallogr. D Struct. Biol. 74, 239 - 255 (2018). doi:10.1107/S2059798318002425
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- **Likelihood based direct phasing with low-dose X-rays.** T. Weiss, P.V. Afonine, P.D. Adams, and A. Brunger, Acta Cryst. (2018).
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- **Chemical fingerprinting of protein complexes by cross-linking and mass spectrometry.** P.D. Adams, A.K. Arora, D.R. Garfinkel, D.M. Matyszewski, N.W. Moriarty, R.I. Sarni, W.A. Yehudi, Nature Communications 9, 1075 (2018).
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- **Highly accurate protein structure prediction with AlphaFold.** J. Jumper, R. Evans, A. Pritzel, T. Green, M. Figurnov, O. Ronneberger, K. Tunyasuvunakool, R. Bates, A. Zidek, A. Potapenko, A. Bridgland, C. Meyer, S.A.A. Kohl, A.J. Ballard, A. Cowie, B. Romera-Paredes, S. Nikolov, R. Jain, J. Adler, T. Back, S. Petersen, D. Reiman, E. Clancy, M. Zielinski, M. Steinegger, M. Pacholska, T. Berghammer, S. Bodenstein, D. Silver, O. Vinyals, A.W. Senior, K. Kavukcuoglu, P. Kohli, D. Hassabis, Nature 596, 583-589 (2021).
- **Cryo-EM map improvement and protein model building using deep learning.** D. Terwilliger, T.C. Terwilliger, R. Dyer, A.M. Oyeyemi, P.V. Afonine, P.D. Adams, Nature Methods (2021).
- **Efficient target-based and local scoring for full-length protein models.** T.C. Terwilliger, P.V. Afonine, N.W. Moriarty, P.D. Adams, Acta Cryst. D 77, 1 - 6 (2021).
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Phenix *Python-based Hierarchical Rhombohedral for Integrated Bioinformatics*

Putting the best parts of several maps together with combine_focused_maps

Author(s)

Tom Terwilliger, phenix.combine_focused_maps Tom Terwilliger

Purpose

The macro combine_focused_maps uses tools being developed to place a model in several maps. It then uses information about the quality of the model in each map to select the best parts of each map and create a composite map.

Usage

How combine_focused_maps works:

Combine focused maps uses the PI of chains in a model to each map to identify the correspondence between chains in the model and regions in the map. Information from the model is used to select the best parts of the map, starting at one

If the model will be used for model improvement, you can create a single chain. The model will be placed in several different places in the map, and the best parts of the map will be used to create a composite map. The model will be improved in the composite map, and then it will be used to place a new model in the map and the process will be repeated.

If the maps are very different, then you will need to provide more than one chain in the model. For example, if the maps are very different, then you will need to provide one chain for each map. The models should all be fit to the same asymmetric unit. The best parts of each map will be used to create a composite map. The models should all be fitted to the same asymmetric unit, and the composite map will be in the same asymmetric unit.

Since a set of models is used as a model for the map, the chain identifiers in the model are used to assign a set of chain in each model to segments. This correlation is calculated in a special way. It is scalable of all the atoms in the chain, and it is not affected by the number of atoms in the chain. The correlation is calculated in a way that is not affected by the number of atoms in the chain. The

Phenix

Advanced Directed Phenomics for Enhanced Pathogenicity

Merging two models with combine_models

Author(s)

- Jordan, Jordan, Tom Terwilliger

Purpose

This tutorial takes a model and finds pieces of a second model that that improve its fit to density when they are added. The corresponding pieces in the first model

Usage

The main uses of phenix.combine_models are:

- Taking the best parts of a model and merging them to make a new model.
- Finding which parts of a model are most improving agreement from another

How combine_models works:

The main function of combine_models is to take two models and see if one can improve the fit of one model to two different areas. One approach keeps segments in the models intact, and the second applies crossovers within segments.

In the first approach (longer, but separate combination) first, each model is scored based on how well it improves agreement with the other model. The segments are then ranked based on how well they improve agreement. It also includes weights based on whether or segment has been assigned to the sequence and the number of residues in the segment. The segments are then added in order, with the agreement recalculated after each one. If that improves overall agreement, the new segment is accepted if it improves overall fit by a cutoff (default 0.01). Segments that do not improve fit are rejected.

Then the segments are scored in reverse order to create a composite model. As part of a segment that does not improve overall fit may improve fit in a different part of the model, this step may add back some segments.

In the second approach, the segments, excluded if adding a segment does not improve overall fit, are broken up into fixed-length segments and fitting is one-way regions and fragments from other models. Then one by one, the segments are added in order, with the agreement recalculated after each one. If that improves overall agreement, the new segment is accepted if it improves overall fit by a cutoff (default 0.01). Segments that do not improve fit are rejected. Then the segments are scored in reverse order to create a composite model.

The second approach to combine_models starts with two input models. The first model is used as the default, if no improvements are found, and the second model is used to see if it improves the first model. The output is a single model. The output model can be a template for refinement, or it can be used "separately" if the second model is a different conformation or a different domain than the first model.

The fit of the models to density is used to decide which of a pair of fragments is best. In general, the combination of two models is done by taking the best parts of each model. The best parts are determined by how well the combined model (combination of a segment in the source model of the number of residues in each fragment) improves the fit to density. The fit to density is measured by the map-model correlation. The segments are ranked based on density as the properties of the main chain atoms in the segment.

The first approach in combine_models is to take the best segments from the two models, keep all those that improve the fit to density, and add them to the corresponding locations in the first model. In this way the first model has grown into a combination of the two models.

The second approach in combine_models has four main steps, each of which is optional:

- Scoring parts of the input models for crossing over and recombination. In this step allows you to do things like find regions where one model is better than the other, or find regions where one model is better than the average of several models, effectively replacing that segment in a way that one specific.
- Finding points where the two models are interchangeable (crossover points). This is done by calculating the percent similarity in the main chain and considering points in the two models where the main chain is very similar. Crossing over at points where the main chain is very similar is likely to be successful.
- Creating the working model with the second input model, allowing only equal length crossovers. Crossing over between two models of different length is difficult to do without introducing insertions and deletions. Insertions and deletions are not allowed, so this step creates a working model with the same length as the first input model. This working model is created by taking segments from the second model, with the choice switching over between one fragment and the other only at positions where the main chain is very similar (crossover points) and where the segment from the second model improves the fit to density more than the segment from the first model.
- Recombination of the two models. In this step, crossovers are allowed to occur between the working model and the first input model. Crossovers are only allowed at positions where the main chain is very similar (crossover points) and where the segment from the second model improves the fit to density more than the segment from the first model. Crossovers are not allowed in regions where the working model is better than the first input model, so this step can replace some of the segments from the working model with segments from the first input model.

Output files from combine_models

combine_models.pdb - A PDB file with your combined model

Examples

Standard use of combine_models:

The following command runs combine_models. From the command line, you can type:

```
phenix.combine_models pdb_in1=1.pdb
pdb_in2=2.pdb mtz_in=1.mtz
ncs_in=1.ncs
```

You can omit the pdb and mtz and ncs keywords and just type in the files from map_coeffs.mtz, recheck the sequence and ncs files, and the pdb files in the current directory.

Ranking all fragments and picking the best ones:

```
phenix.combine_models pdb_in1=1.pdb
pdb_in2=2.pdb mtz_in=1.mtz ncs_in=1.ncs rank_fragments=True
```

This will rank all fragments in the two input models, keep the best ones, keeping only part of any segment that does not improve overall fit, and write out a combined model.

Relaxing pieces from the two models:

To take first pdb and then see if residues 410-430 of second pdb can improve it, you can type:

```
phenix.combine_models pdb_in1=1.pdb
pdb_in2=2.pdb mtz_in=1.mtz
ncs_in=1.ncs
relax_pieces=True
relax_pieces_in2=410-430
relax_pieces_in1=1-409,431-end
```

Crossing two models that have entirely matched residues:

If you have pdb and ncs and pdb files exactly the same (unless present) and all other if combinations, then you can use the keywords to specify that the two models are identical and that you want to do crossing over. You can overlap crossover points, and so skipping the requirement of sequence. You can type:

```
phenix.combine_models pdb_in1=1.pdb
pdb_in2=2.pdb mtz_in=1.mtz
ncs_in=1.ncs
identical_pdb=True
identical_ncs=True
crossover_only=True
```

Possible Problems

If you are supplying a new key map, running combine_models can require a lot of memory. In this case, you can specify a smaller number of residues in a segment (default 20) with segment_length=20 and also you can specify around how many residues and models and make a local combine map that will require less memory.

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
input_files
  pdb_in1 = None          Input pdb file. This model will be the default output model
                          if no improvements are found. If only one model is given on the
                          command line, it will be used as the first model.
  pdb_in2 = None          Input pdb file. This model will be used if it is expected to be
                          better than the first model in some regions.
  mtz_in = None           Input mtz file. This file will be used to calculate map
                          coefficients and score the models.
  ncs_in = None           Input NCS file with NCS information. If ncs_in=1.ncs is set
                          then 1.ncs will be used as the NCS file. If ncs_in=ncs.ncs is set
                          then ncs.ncs will be used as the NCS file. If ncs_in=1.mtz is set
                          then 1.ncs will be used as the NCS file if 1.mtz is the map_coeffs
                          file. If ncs_in=1.pdb is set then 1.ncs will be used as the NCS
                          file if 1.pdb is the first model.
  map_in = None           Input MTZ file with map coefficients
  map_coeffs_mtz = None   Output MTZ file with map coefficients
  ncs_out = None          Output NCS file (if any) (default: combine_models.ncs)
  pdb_out = None          Output PDB file (default: combine_models.pdb)
  seq_file = None         Input sequence file (optional)
  ncs_file = None         Input NCS file (optional)
  map_file = None         Input map file (optional)
  model_1_weight = None   Weight on model 1 (default: 1.0)
  model_2_weight = None   Weight on model 2 (default: 1.0)
  map_weight = None       Weight on map (default: 1.0)
  ncs_weight = None       Weight on NCS (default: 1.0)
  seq_weight = None       Weight on sequence (default: 1.0)
  segment_length = None   Length of segment (default: 20)
  n_segment = None        Number of segments (default: 100)
  n_segment_2 = None      Number of segments in second round (default: 100)
  max_gap_length = None   Maximum gap length (default: 3)
  max_delta_rms = None    Maximum delta RMS (default: 0.5)
  max_rms_to_accept = None  Maximum acceptable RMS of model in superposition (default:
                          1.0) (if RMS is greater than this, segment will be not be used)
  min_overlap_fraction_for_rms = None  Minimum overlap fraction for RMS calculation
                          (default: 0.5) (if overlap is less than this, RMS will be not
                          be used)
  min_good_points_with_ncs = None  Minimum number of good points with NCS (default: 100)
  min_good_points_no_ncs = None  Minimum number of good points without NCS (default:
                          100)
  min_fraction_good_points_with_ncs = None  Minimum fraction of good points with NCS
                          (default: 0.5)
  min_fraction_good_points_no_ncs = None  Minimum fraction of good points without NCS
                          (default: 0.5)
  min_fraction_overlap_with_ncs = None  Minimum fraction of overlap with NCS (default:
                          0.5)
  min_fraction_overlap_no_ncs = None  Minimum fraction of overlap without NCS (default:
                          0.5)
  min_fraction_good_points_for_rms = None  Minimum fraction of good points for RMS
                          calculation (default: 0.5)
  min_residues_in_alignment = None  Minimum number of residues in alignment (default:
                          10)
  weight_by_rms = None    Weight by RMS (default: yes)
  weight_by_gaps = None   Weight by gaps (default: yes)
  weight_by_length = None Weight by length (default: yes)
  n_segment_1 = None      Number of segments in first round (default:
                          n_segment/2)
  n_segment_2 = None      Number of segments in second round (default:
                          n_segment/2)
  n_segment_3 = None      Number of segments in third round (default: n_segment/2)
  max_gap_length_1 = None Maximum gap length in first round (default: 3)
  max_gap_length_2 = None Maximum gap length in second round (default: 3)
  max_gap_length_3 = None Maximum gap length in third round (default: 3)
  max_delta_rms_1 = None  Maximum delta RMS in first round (default: 0.5)
  max_delta_rms_2 = None  Maximum delta RMS in second round (default: 0.5)
  max_delta_rms_3 = None  Maximum delta RMS in third round (default: 0.5)
  max_rms_to_accept_1 = None  Maximum acceptable RMS of model in superposition in first
                          round (default: 1.0) (if RMS is greater than this, segment
                          will be not be used)
  max_rms_to_accept_2 = None  Maximum acceptable RMS of model in superposition in second
                          round (default: 1.0) (if RMS is greater than this, segment
                          will be not be used)
  max_rms_to_accept_3 = None  Maximum acceptable RMS of model in superposition in third
                          round (default: 1.0) (if RMS is greater than this, segment
                          will be not be used)
  min_overlap_1 = None    Minimum overlap in first round (default: 0.5)
  min_overlap_2 = None    Minimum overlap in second round (default: 0.5)
  min_overlap_3 = None    Minimum overlap in third round (default: 0.5)
  min_good_points_1 = None  Minimum number of good points in first round (default:
                          100)
  min_good_points_2 = None  Minimum number of good points in second round (default:
                          100)
  min_good_points_3 = None  Minimum number of good points in third round (default:
                          100)
  min_fraction_good_points_1 = None  Minimum fraction of good points in first round
                          (default: 0.5)
  min_fraction_good_points_2 = None  Minimum fraction of good points in second round
                          (default: 0.5)
  min_fraction_good_points_3 = None  Minimum fraction of good points in third round
                          (default: 0.5)
  min_fraction_overlap_1 = None  Minimum fraction of overlap in first round (default:
                          0.5)
  min_fraction_overlap_2 = None  Minimum fraction of overlap in second round (default:
                          0.5)
  min_fraction_overlap_3 = None  Minimum fraction of overlap in third round (default:
                          0.5)
  min_residues_in_alignment_1 = None  Minimum number of residues in alignment in first
                          round (default: 10)
  min_residues_in_alignment_2 = None  Minimum number of residues in alignment in second
                          round (default: 10)
  min_residues_in_alignment_3 = None  Minimum number of residues in alignment in third
                          round (default: 10)
  weight_by_rms_1 = None  Weight by RMS in first round (default: yes)
  weight_by_rms_2 = None  Weight by RMS in second round (default: yes)
  weight_by_rms_3 = None  Weight by RMS in third round (default: yes)
  weight_by_gaps_1 = None Weight by gaps in first round (default: yes)
  weight_by_gaps_2 = None Weight by gaps in second round (default: yes)
  weight_by_gaps_3 = None Weight by gaps in third round (default: yes)
  weight_by_length_1 = None  Weight by length in first round (default: yes)
  weight_by_length_2 = None  Weight by length in second round (default: yes)
  weight_by_length_3 = None  Weight by length in third round (default: yes)
  remove_pieces_with_fragments_1 = None  Remove pieces with fragments in first round
                          (default: yes)
  remove_pieces_with_fragments_2 = None  Remove pieces with fragments in second round
                          (default: yes)
  remove_pieces_with_fragments_3 = None  Remove pieces with fragments in third round
                          (default: yes)
  keep_fragments = None   Keep fragments (default: yes)
  keep_segments = None    Keep segments (default: yes)
  keep_fragments_1 = None Keep fragments in first round (default: yes)
  keep_fragments_2 = None Keep fragments in second round (default: yes)
  keep_fragments_3 = None Keep fragments in third round (default: yes)
  keep_segments_1 = None  Keep segments in first round (default: yes)
  keep_segments_2 = None  Keep segments in second round (default: yes)
  keep_segments_3 = None  Keep segments in third round (default: yes)
  rank_fragments = None   Rank fragments (default: yes)
  rank_fragments_1 = None Rank fragments in first round (default: yes)
  rank_fragments_2 = None Rank fragments in second round (default: yes)
  rank_fragments_3 = None Rank fragments in third round (default: yes)
  rank_by_length = None   Rank by length (default: yes)
  rank_by_length_1 = None Rank by length in first round (default: yes)
  rank_by_length_2 = None Rank by length in second round (default: yes)
  rank_by_length_3 = None Rank by length in third round (default: yes)
  rank_by_rms = None      Rank by RMS (default: yes)
  rank_by_rms_1 = None    Rank by RMS in first round (default: yes)
  rank_by_rms_2 = None    Rank by RMS in second round (default: yes)
  rank_by_rms_3 = None    Rank by RMS in third round (default: yes)
  rank_by_gaps = None     Rank by gaps (default: yes)
  rank_by_gaps_1 = None   Rank by gaps in first round (default: yes)
  rank_by_gaps_2 = None   Rank by gaps in second round (default: yes)
  rank_by_gaps_3 = None   Rank by gaps in third round (default: yes)
  rank_by_fraction_of_model = None  Rank by fraction of model (default: yes)
  rank_by_fraction_of_model_1 = None  Rank by fraction of model in first round
                          (default: yes)
  rank_by_fraction_of_model_2 = None  Rank by fraction of model in second round
                          (default: yes)
  rank_by_fraction_of_model_3 = None  Rank by fraction of model in third round
                          (default: yes)
  rank_by_fraction_of_sequence = None  Rank by fraction of sequence (default: yes)
  rank_by_fraction_of_sequence_1 = None  Rank by fraction of sequence in first round
                          (default: yes)
  rank_by_fraction_of_sequence_2 = None  Rank by fraction of sequence in second round
                          (default: yes)
  rank_by_fraction_of_sequence_3 = None  Rank by fraction of sequence in third round
                          (default: yes)
  relax_pieces = False    Relax pieces (default: no)
  relax_pieces_in1 = None Relax pieces in first model (default: all)
  relax_pieces_in2 = None Relax pieces in second model (default: all)
  relax_fragments = False Relax fragments (default: no)
  relax_fragments_in1 = None  Relax fragments in first model (default: all)
  relax_fragments_in2 = None  Relax fragments in second model (default: all)
  relax_segments = False  Relax segments (default: no)
  relax_segments_in1 = None  Relax segments in first model (default: all)
  relax_segments_in2 = None  Relax segments in second model (default: all)
  relax_segment_length = None  Relax segment length (default: 20)
  relax_segment_1 = None  Relax segment 1 (default: no)
  relax_segment_2 = None  Relax segment 2 (default: no)
  relax_segment_3 = None  Relax segment 3 (default: no)
  relax_both_models = False  Relax both models (default: no)
  relax_in_chunks = False Relax in chunks (default: no)
  relax_in_chunks_fraction = None  Relax in chunks fraction (default: 0.5)
  relax_in_chunks_fraction_1 = None  Relax in chunks fraction 1 (default: 0.5)
  relax_in_chunks_fraction_2 = None  Relax in chunks fraction 2 (default: 0.5)
  relax_in_chunks_fraction_3 = None  Relax in chunks fraction 3 (default: 0.5)
  n_cycle_relax = None    Number of cycles to relax (default: 1)
  n_cycle_relax_1 = None  Number of cycles to relax 1 (default: 1)
  n_cycle_relax_2 = None  Number of cycles to relax 2 (default: 1)
  n_cycle_relax_3 = None  Number of cycles to relax 3 (default: 1)
  n_cycle_relax_all = None  Number of cycles to relax all (default: 1)
  n_cycle_relax_all_1 = None  Number of cycles to relax all 1 (default: 1)
  n_cycle_relax_all_2 = None  Number of cycles to relax all 2 (default: 1)
  n_cycle_relax_all_3 = None  Number of cycles to relax all 3 (default: 1)
  n_cycle_relax_with_ncs = None  Number of cycles to relax with ncs (default: 1)
  n_cycle_relax_with_ncs_1 = None  Number of cycles to relax with ncs 1 (default: 1)
  n_cycle_relax_with_ncs_2 = None  Number of cycles to relax with ncs 2 (default: 1)
  n_cycle_relax_with_ncs_3 = None  Number of cycles to relax with ncs 3 (default: 1)
  n_cycle_relax_with_ncs_all = None  Number of cycles to relax with ncs all (default:
                          1)
  n_cycle_relax_with_ncs_all_1 = None  Number of cycles to relax with ncs all 1
                          (default: 1)
  n_cycle_relax_with_ncs_all_2 = None  Number of cycles to relax with ncs all 2
                          (default: 1)
  n_cycle_relax_with_ncs_all_3 = None  Number of cycles to relax with ncs all 3
                          (default: 1)
  n_cycle_rsr = None      Number of cycles to rsr (default: 1)
  n_cycle_rsr_1 = None    Number of cycles to rsr 1 (default: 1)
  n_cycle_rsr_2 = None    Number of cycles to rsr 2 (default: 1)
  n_cycle_rsr_3 = None    Number of cycles to rsr 3 (default: 1)
  n_cycle_rsr_all = None  Number of cycles to rsr all (default: 1)
  n_cycle_rsr_all_1 = None  Number of cycles to rsr all 1 (default: 1)
  n_cycle_rsr_all_2 = None  Number of cycles to rsr all 2 (default: 1)
  n_cycle_rsr_all_3 = None  Number of cycles to rsr all 3 (default: 1)
  n_cycle_rsr_with_ncs = None  Number of cycles to rsr with ncs (default: 1)
  n_cycle_rsr_with_ncs_1 = None  Number of cycles to rsr with ncs 1 (default: 1)
  n_cycle_rsr_with_ncs_2 = None  Number of cycles to rsr with ncs 2 (default: 1)
  n_cycle_rsr_with_ncs_3 = None  Number of cycles to rsr with ncs 3 (default: 1)
  n_cycle_rsr_with_ncs_all = None  Number of cycles to rsr with ncs all (default:
                          1)
  n_cycle_rsr_with_ncs_all_1 = None  Number of cycles to rsr with ncs all 1
                          (default: 1)
  n_cycle_rsr_with_ncs_all_2 = None  Number of cycles to rsr with ncs all 2
                          (default: 1)
  n_cycle_rsr_with_ncs_all_3 = None  Number of cycles to rsr with ncs all 3
                          (default: 1)
  keep_ncs = False        Keep ncs (default: no)
  keep_ncs_1 = None       Keep ncs 1 (default: no)
  keep_ncs_2 = None       Keep ncs 2 (default: no)
  keep_ncs_3 = None       Keep ncs 3 (default: no)
  keep_ncs_all = None     Keep ncs all (default: no)
  keep_ncs_all_1 = None   Keep ncs all 1 (default: no)
  keep_ncs_all_2 = None   Keep ncs all 2 (default: no)
  keep_ncs_all_3 = None   Keep ncs all 3 (default: no)
  keep_ncs_with_ref = None  Keep ncs with ref (default: no)
  keep_ncs_with_ref_1 = None  Keep ncs with ref 1 (default: no)
  keep_ncs_with_ref_2 = None  Keep ncs with ref 2 (default: no)
  keep_ncs_with_ref_3 = None  Keep ncs with ref 3 (default: no)
  keep_ncs_with_ref_all = None  Keep ncs with ref all (default: no)
  keep_ncs_with_ref_all_1 = None  Keep ncs with ref all 1 (default: no)
  keep_ncs_with_ref_all_2 = None  Keep ncs with ref all 2 (default: no)
  keep_ncs_with_ref_all_3 = None  Keep ncs with ref all 3 (default: no)
  keep_ncs_with_ref_with_ncs = None  Keep ncs with ref with ncs (default: no)
  keep_ncs_with_ref_with_ncs_1 = None  Keep ncs with ref with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_2 = None  Keep ncs with ref with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_3 = None  Keep ncs with ref with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all = None  Keep ncs with ref with ncs all (default:
                          no)
  keep_ncs_with_ref_with_ncs_all_1 = None  Keep ncs with ref with ncs all 1
                          (default: no)
  keep_ncs_with_ref_with_ncs_all_2 = None  Keep ncs with ref with ncs all 2
                          (default: no)
  keep_ncs_with_ref_with_ncs_all_3 = None  Keep ncs with ref with ncs all 3
                          (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs = None  Keep ncs with ref with ncs all with
                          ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_1 = None  Keep ncs with ref with ncs all with
                          ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_2 = None  Keep ncs with ref with ncs all with
                          ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_3 = None  Keep ncs with ref with ncs all with
                          ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs = None  Keep ncs with ref with ncs
                          all with ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_1 = None  Keep ncs with ref with
                          ncs all with ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_2 = None  Keep ncs with ref with
                          ncs all with ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_3 = None  Keep ncs with ref with
                          ncs all with ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs = None  Keep ncs with ref
                          with ncs all with ncs with ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_1 = None  Keep ncs with
                          ref with ncs all with ncs with ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_2 = None  Keep ncs with
                          ref with ncs all with ncs with ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_3 = None  Keep ncs with
                          ref with ncs all with ncs with ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs = None  Keep ncs
                          with ref with ncs all with ncs with ncs with ncs with ncs
                          (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_1 = None  Keep
                          ncs with ref with ncs all with ncs with ncs with ncs with
                          ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_2 = None  Keep
                          ncs with ref with ncs all with ncs with ncs with ncs with
                          ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_3 = None  Keep
                          ncs with ref with ncs all with ncs with ncs with ncs with
                          ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs = None
                          Keep ncs with ref with ncs all with ncs with ncs with ncs
                          with ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_1 = None
                          Keep ncs with ref with ncs all with ncs with ncs with ncs
                          with ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_2 = None
                          Keep ncs with ref with ncs all with ncs with ncs with ncs
                          with ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_3 = None
                          Keep ncs with ref with ncs all with ncs with ncs with ncs
                          with ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _1 = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _2 = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _3 = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs
                          (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_1 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_2 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_3 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_1 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_2 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_3 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_1 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_2 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_3 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_with_ncs = None  Keep ncs with ref with
                          ncs all with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_1 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_2 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_3 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _1 = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _2 = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _3 = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_1 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_2 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_3 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_1 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_2 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_3 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _1 = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _2 = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _3 = None  Keep ncs with ref with ncs all with ncs with ncs
                          with ncs with ncs with ncs with ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_1 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_2 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_3 = None  Keep ncs with ref with ncs all with ncs
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs 3 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_1 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs 1 (default: no)
  keep_ncs_with_ref_with_ncs_all_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs_with_ncs
                          _with_ncs_with_ncs_2 = None  Keep ncs with ref with ncs all
                          with ncs with ncs with ncs with ncs with ncs with ncs with
                          ncs with ncs with ncs 2 (default: no)
  keep_ncs_with_ref_with_nc
```

composite_smtt_map

Python-based Reactive Modules for Crystal Kinetics

Generating a composite smtt *map*

Contents

- Overview
- Running the program
- Stop-smtt mode
- Other options
- References
- List of all available keywords

Overview

This program is used to generate a composite smtt map combining the smtt contents of the unit cell, generated by computing a number of smtt maps covering specific regions, and combining the scale around the contained regions. This allows for a single smtt map to be used for simulations of systems with multiple different types of local environments. Because this is significantly faster than computing a single smtt map it is not recommended if you are only interested in one type of local environment, however if you are interested in multiple types of local environments it may be special use case instead procedures or create nodes to link the systems.

The program `smtt_composite.py` may be used to generate these maps. Internally, it attempts to move from the specified smtt maps to the composite smtt map using the following steps, which are described in more detail below:

- **with associated computing**, which approximate removes vertices lost in the period modes
- **with minimization only**, without approximate
- **stop-smtt mode**, which stops after the initial smtt maps are created alone, but performs no iterative minimization or approximate removal

The final option is the default, since it is also fast and efficient, the last modes are recommended running with minimized timeseq without this may be more problematic for especially poor and/or low resolution structures.

Running the program

Execution of the program is very similar to running phenix.refine:

```
phenix.composite_smtt map model.pdb data=data.hkl type=f,sigf,r free=free.hkl
```

The composite smtt map files will be created in the dir. Because the program is intended to be automatic and reproducible, it does not automatically overwrite previous output files. Instead, it will stop with an error if any output files are found in the dir. This can be overwritten using the `overwrite` option, or the output directory can be changed using the `dir` option. The output files include the composite smtt map, the minimized model, and the refinement parameters.

You may request a **a** parameter combination of maps using the same map but stored as alternates in Phenix. This is a single smtt map with multiple sets of parameters. This is specified using `a=1,2,3` or `a=1-3`. If no `a` is specified, the default is `a=1`. Alternate maps, if any, are stored using the name of alternate in the output files, for example `composite_smtt_map_alternate.map`. The alternate number is also included in the output log (or STDOUT) accessing to dim available as an option.

Parameters for the smtt map can be specified using the `parameters` option, or by separate `smtt` keywords. If `parameters` is used, the file specified by `parameters` is read in, using defaults for `smtt` for any parameters not specified in the file. Alternate parameters for the alternate maps can also be specified, with by default be searched in their working directory for a file with the same name as the working parameter file, but with `_alternate` appended before the extension. Alternate parameters for the alternate maps may be turned off by setting the keyword `no_alternate_maps` to `True`, or a value other than `None` and `False`.

The program will parallelize over multi-core systems or managed clusters (including but not limited, MPI, qsub, and slurm) if the `nproc` option is set to a value greater than 1. Parallelization is done over the smtt maps, and the number of processes used will be the minimum of the number of smtt maps and the specified `nproc`. Because of this, it is recommended to use `nproc` equal to the number of smtt maps, which is 27 by default, or 8 if `stop-smtt` mode is used.

Because composed of single MTZ files, separate `compute` and `apply` to `timeseq`, one may specify a predicted file name using the keyword the keyword `output.file_name`. This will convert predicted and stored for each map in the `dir` directory, and combine into a single file. This will convert predicted and stored for each map in the `dir` directory, and combine into a single file. This will convert predicted and stored for each map in the `dir` directory, and combine into a single file. This is interpretable using the easy-to-use `tutorial` or `tlsmd` or `tlsmd-cli` tools found in the `tlsmd` repo manually.

Stop-smtt mode

The program can also be used to generate a single smtt map for a single region. The function for this procedure is contained in `smtt_composite.stop_smtt_map()`. This function takes the same inputs as `run()`. This is recommended because it setting up a single cells run manually, or with a simplified timeseq.

Other options

There are several other options in Phenix with similar features:

- `mmtbx.tls` an older implementation of this method. A more powerful approach is to generate an "alternate-level" smtt map (Terwilliger et al. 2006), which models the structure instead of the cell.
- `mmtbx.tls.tlsmd_analysis` and `mmtbx.tls.tlsmd_output` are tools for analyzing and visualizing the results of `mmtbx.tls`, and `mmtbx.tls.tlsmd` is a combined tool. The output which most of the composite smtt map tools generate should work with these tools.
- `mmtbx.tls.qscore` can generate phenix smtt maps without refinement.

References

- **Phenix tlsmd in macromolecular crystal structures**, P. Grosh, S.M. Kerr, and E.J. Bourgeois. Acta Cryst. D Struct. Biol. 2018.
- **Iterative-TLS (ITLS): a way improvement by iterative model building and refinement without a priori TLS decomposition**. Urzhumtsev, A., Afonine, P.V., Lunin, V.Y., Terwilliger, T.C., Adams, P.D. Acta Cryst. D 65, 307-317 (2009).
- **Rigid-body refinement of protein and RNA molecules by translation, libration, screw (TLS) parameters**. Winn, J.D., Ashton, A.W., Briggs, P.J. Acta Cryst. D 61, 632-637 (2005).
- **Generalized Scaling, Weighting, and Partial Molecular Replacement for phase refinement**. Ed Wolska, K.S. Bruno, T.C. Terwilliger. Acta Cryst. D 61, 1755-1762 (2005).
- **Phenix: a comprehensive python-based system for macromolecular structure solution**. P.D. Adams, P.V. Afonine, G. Bunkóczi, V.B. Chen, I.W. Davis, N. Echols, J.J. Headd, L.-W. Hung, G.J. Kapral, R.W. Grosse-Kunstleve, A.J. McCoy, N.W. Moriarty, R. Oeffner, R.J. Read, D.C. Richardson, J.S. Richardson, T.C. Terwilliger, P.H. Zwart. Acta Cryst. D 66, 213-221 (2010).

List of all available keywords

(Light-phenix-command: dev.composite_smtt_map.)

Phenis *Reflection Heuristics Mechanism for Integrated Bibliography*

Generating alternative conformations switching a map with create_slt_conf

Author(s):

- Jones, T. Alwyn Tom Terwilliger, Paul Adams, Pavel Afonine, Randy Read, Gerard Bricogne

Purpose

The purpose of create_slt_conf is to create alternate side-chain conformations for a structure using very high resolution data. Normally 1.5 is about the lowest resolution that is useful.

The output file is a pdb file in which the side-chain conformations present in a structure, residues that have no alternate side-chain conformations, and residues that have only one alternate side-chain conformation, are left unchanged. Residues with more than two alternate side-chain conformations are left unchanged. Residues with two alternate side-chain conformations are given occupancies of 0.5 and the side-chain conformations are given the same B-factor as the original side-chain conformation.

Note that the model that is produced is not intended to be a final model, rather it is a model that has some alternate side-chain conformations. It is recommended that you use the conformations in the output model as suggestions for your model.

How create_slt_conf works:

Generating alternative conformations:

The starting point for create_slt_conf is normally a model with a single conformation (i.e.A or blank).

The program looks for a number of possible conformations for each side-chain based on the current model and the 2-fold data in a mtz file.

For A-alone, a blank (50% chance) is created. This map is expected to show conformations that are not represented in the current model, but are present in the data.

In other words, alternate conformations for all side-chain rotamers and for the backbone are created in a manner that is independent of the current model. The idea is that the data will show alternate conformations that are not in the current model and that are different from the current conformer or that positions in shapes of alternate conformations are different from those in the current conformer. Alternate conformations for side-chain rotamers are generated. The side-chain alternate conformations are then scored using a map-model map-correlation-type function. The side-chain rotamers are then ordered by the scores and the top two are selected. The rotamers are then fit into the A-alone or blank map. The result is that one is a pair of rotamers, the original one and that fit to the alternate conformation. The B-factor of the alternate conformation is set to the B-factor of the original side-chain conformation.

If alternate sites, one and two rotamers were added to a residue that already had a side-chain with two alternate conformations, the residue is left unchanged. Residues with three alternate conformations are left unchanged.

Optimizing assignment of side-chain conformers to models:

The first step is to create all side-chains and all rotamers and then to select the good conformers and the good rotamers. The goal is to find the best set of side-chain conformations that are consistent with the side-chain conformations as seen in all solutions. The challenging part of this step is arranging the side-chain conformations so that they are consistent with the side-chain conformations in other solutions.

The procedure used is to generate a tree of all allowed side-chain conformer possibly, to score each branch, then to select the best branch and then to generate a pruned tree of side-chain conformer models. The procedure is complicated by the fact that the side-chain conformations are not independent of the backbone conformations and of the side-chain conformations of other residues.

Scoring function:

The scoring function used to score side-chain conformers is the Kolkman-Jones-Terwilliger scoring function. This scoring function is a function of the side-chain conformer and the backbone conformer. It is based on the expected electron density of a model. The scoring function requires a refined model, an unrefined model and a map. The scoring function is described in the Kolkman-Jones-Terwilliger paper.

The scoring function is also calculated on a per-residue basis. This per-residue score is the Kolkman-Jones-Terwilliger scoring function calculated for each residue. This score is used to order side-chain rotamers and to select the best side-chain conformer. The per-residue score is also used to determine when side-chain conformers are seen and when side-chain and alternate conformers are seen in all solutions. The per-residue score is also used to determine when side-chain conformers are seen in all solutions.

Probabilistic estimation of score for a new arrangement of side chain:

To reduce the number of rotamers that need to be fully scored, a procedure for a probabilistic estimation of the score for a new arrangement of side-chain conformers is used. The probabilistic estimation of the score is based on the sum of the most significant (smallest) distance between residues left to right residue (sequence of residues) and the current residue.

The starting point for the probabilistic is a set of scored models with one conformer per residue. The probabilistic estimation of the score for a new arrangement of side-chain conformers is based on the sum of the group, pair, triplet, quadruplet, etc. The probabilistic estimation of the score for a new arrangement of side-chain conformers is based on the sum of the group, pair, triplet, quadruplet, etc. The probabilistic estimation of the score for a new arrangement of side-chain conformers is based on the sum of the group, pair, triplet, quadruplet, etc. The probabilistic estimation of the score for a new arrangement of side-chain conformers is based on the sum of the group, pair, triplet, quadruplet, etc.

With these procedures for the effects of changes in alternative conformations at one residue on the context of other residues, the probabilistic estimation of the score for a new arrangement of side-chain conformers is calculated. The score for the new arrangement of side-chain is a function of the sum of the group, pair, triplet, quadruplet, etc. The probabilistic estimation of the score for a new arrangement of side-chain conformers. The score is a function of the sum of the group, pair, triplet, quadruplet, etc.

Recombination procedure:

The recombination procedure is adapted from Jones' recombination. The goal is to find a set of side-chain conformers that are consistent with the side-chain conformers in all solutions. The procedure is a tree search. The procedure is a tree search. The procedure is a tree search

create_maps

Phase-based Macromolecular Crystallography

Creating maps using the Phenix GUI

Contents

- Intro: Create Map2 GUI
- Guidelines for use
- References

Because of the differences in calculation method and input data, there is no single unified interface for creating any electron density maps. Instead, separate programs are grouped together in the main GUI. For most maps, a reflection file and a PDB file are required, and the program defaults to the most common maps, both DFC and DFo difference maps, and 2mFo-DFc and mFo-DFc maps. Other maps are available in the drop down menu. Details on the Create Map2 GUI, and how to use it, are given below. For more information on the Phenix Map2 program, see the Phenix documentation. Note that the GUI uses the PDB file only for grouping it together with the reflection file, and does not utilize it to scale the PDB data for grouping it together.

The "Create Maps" GUI

This is accessed by selecting Map2 from a column of programs with prefix Create. Many user-defined map types are possible, but the program defaults to the most common ones, both DFC and mFo-DFc difference maps, and standard weighted maps are available in the drop down menu.

The pre-defined maps include all common likelihood weighted difference maps, anomalous difference maps, and standard weighted maps. Other maps are available by selecting from a drop down menu in the Map type field. Some maps require an input file, which can be selected using the browse button, or a global number for those already loaded in the GUI can be given in the Map coefficients (1) or Map coefficients (2) fields.

By default the program only generates an MTZ file containing the map coefficients, but you may separately specify a CCP4 map file to be created, and a resolution limit for the output map. Note that the CCP4 map file is oversampled, so input these parameters only if you are generating a map for a specific CCP4 format file or if you want to limit the resolution of the output map for some reason.

Guidelines for use

- The quality may be heavily influenced by reflections that are missing due to errors in data processing, or because they were not measured. Missing reflections can be filled in using the Fill missing maps in a field option. Alternatively, the default maps output by phenix.refine and phenix.phaser do not have missing reflections, and these can be used instead. Missing reflections can also be recovered using the same phase and an alternative normal-mode based amplitude, using the Apply B factor sharpening option. Note that this option also applies amplitude-dependent blurring, so use with caution.
- Resolution limits can be used to remove low resolution data, e.g. to remove the solvent-ordered shell, or to remove high resolution data if the data are very noisy.
- If you are using Phenix Refine and the Refinement GUI to "Refine", alternatively, have it set to output the map coefficients and then use the Refinement GUI to "Refine".

References

- **Averaged Fo(H) maps: less noise, more signal... and probably less bias.** J. Fejfarova, P.V. Afonine, G. Sumai, P.H. Zwart, P.D. Adams, Acta Crystallogr D Struct Biol Crystallogr **[73]**, 821-32 (2017)

cryo_fit

Phenix *Python-based Hierarchical Environment for Integrated Xtallography*

Cryo_fit: Fitting Structure to Cryo-EM Map Using MD Simulation

Contents

- Overview
- Introduction
- How to Fit Cryo-EM Maps
- Advantages
- How Cryo_fit Works
- How to Run Cryo_fit
- FAQ
- Reference

Overview

Cryo_fit by Dimitrios Lamprakis (protein and nucleic acid) structures to cryo-EM maps using molecular dynamics (MD) simulation.

Introduction

Cryo_fit is an automated cryo-EM density fitting program using MD simulation to guide models into maps. Cryo_fit produces all atom models highly consistent with the EM density and is easily used to optimize models for further refinement and interpretation. Cryo_fit requires a cryo-EM map, a starting model, and a sequence file. The starting model can be a homologous structure, an AlphaFold prediction, or a manually created structure. Cryo_fit uses OpenMM to perform molecular dynamics (MD) simulations. The simulation includes the cryo-EM density as a force, guiding the atoms into the density while maintaining bonds, angles, rotamers, Ramachandran, secondary structure, chiralities, and nonbonded potentials allowing the preservation of stereochemistry information. In addition, secondary structure restraints can optionally be applied to the protein or additional restraints on contacts to help minimize chain crossing into fitting proteins.

How to Fit Cryo-EM Maps

Advantages

Fast speed

- Uses a reduced model (reduced energy function)
- Runs on a single laptop (several hours for a ribosome modeling without the need for GPU) instead of thousands of cores.

Preserving stereochemistry

- Uses secondary and tertiary contact restraints
- Uses native contact potentials

before (A) and after (B) Cryo_fit
(Kimanius et al. Nathcom Dec 2015)

Example of MDFF: Human ribosome (Budkevich, et al., Cell 2014)

Example of MDFF: Yeast cytoplasmic 80S ribosome translocation (Ratje et al., Nature 2010)

How Cryo_fit Works

How to Run Cryo_fit

See the tutorial notes for cryo_fit.

FAQ

See the FAQ for Cryo_fit.

Reference

1. Nature Communications Biology, Volume 108, 2019; Paula A. D. Cruz, TR. Desfosses/Nature of Tunable Fitting for cryo-EM

Phonia Active Learning Microtubule Movement for Integrated Molecularity

Cryo_fit2: Fitting to a Cryo-EM Map using Phonia Dynamics

Contents

- Note
- Author
- When cryo_fit1 and cryo_fit2 are useful?
- When cryo_fit2 is useful?
- When cryo_fit2 is more useful than cryo_fit1?
- Theory
- How to install
- How to Run Cryo_fit2
- FAQ
- Limitation

Note

cryo_fit2 is under active development.

Contact to use cryo_fit2 instead.

Author

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When cryo_fit1 and cryo_fit2 are useful?

See the Wiki page cryo_fit1 and cryo_fit2 are useful?.

When cryo_fit2 is useful?

See the Wiki page cryo_fit2 is useful?.

When cryo_fit2 is more useful than cryo_fit1?

See the Wiki page cryo_fit2 is more useful than cryo_fit1?.

Theory

- Phonia Dynamics uses Langevin dynamics.
- Langevin dynamics is used in cryo_fit2 instead to minimize the object function Γ (Γ = Phonia Dynamics Potential + Cryo-EM Potential).
- In cryo_fit2, mass is the EM-fitting weight and so is a parameter keeping weight.

How to install

See the Installation guide for cryo_fit2.

How to Run Cryo_fit2

See the tutorial guide for cryo_fit2

FAQ

See the cryo_fit2 FAQ

Limitation

- Cryo_fit2 is based on an electrostatic interaction. Therefore, it does not fully capture all physical forces.
  - See the Wiki page Limitation for details.
  - Future versions will add cryo-electrostatic interaction so that molecular dynamics simulation runs faster.

Phenix

Python based Hierarchical Environment for Integrated Bioinformatics

Cutting density out of a map with cut_out_density

- Syntax
- Purpose
- Usage
- How cut_out_density works
- Output files from cut_out_density
- List of all available keywords

Author(s):

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Purpose:

The program cut_out_density cut out a map and writes an EXTC file in space group P1 with new coefficients for the cut out density. The density map is calculated from new coefficients supplied as an input EXTC file. The region to be cut out can be specified by a PDB file that defines the region to be cut out, by the center of a PDB file that is a single point in cut out density, or around a specified point. Alternatively the region can be specified by a PDB file, by the center of a PDB file, or around a specified point, and a specified radius around the specified region. The density can optionally be shifted to have a mean density of zero. The region outside the cut out region always will have a density of zero. The output coordinates are shifted to be consistent with the original coordinates in the input EXTC file (unless the cut out coordinates). The resolution of the cut out map can also be specified (the input map will be truncated at the specified resolution). The output EXTC file can optionally be converted to the CCP4 formatted MAP.

Usage:

The main code of phenix.cut_out_density are:

- Cutting out a small part of a map and molecule to work on independently of the rest of the structure. This allows you to work on a small part of a large structure without having to deal with the rest of the structure. The program can cut out the unit cell and space group coordinates of the molecule that are in a specified region of the unit cell. The output coordinates are shifted to be consistent with the original coordinates in the input PDB file (unless the cut out coordinates).

How cut_out_density works:

cut_out_density assumes that you are supplying map coefficients and coordinates in map. Then it creates a map, cuts out the density, and writes out the new map coefficients. The output coordinates are shifted to be consistent with the origin of your density around it. The density is zero map at the corner (so specify a field outside of the origin in the input EXTC file if you want to have a non-zero density at the corner).

You can optionally specify the region to be cut out as a box, a sphere, or a region defined by all points within a specified distance of points in a PDB file.

You can optionally move the center of the region to be cut out with its coordinates, or by the centroid of a PDB file that is there.

If you specify no input PDB file, you can use a selection string to select any part of that model (i.e., one domain or all ligand molecules, or all water molecules, or all residues with a specified name).

If you specify an input PDB file, then the selected atoms from that file will be offset to match the new map and written out.

As a convenience, you can in addition, a PDB file back to the original position in your original model as well.

Output files from cut_out_density

cutout.ccp4: An EXTC MAP with your cut out density in space group P1.

cutout.pdb: A PDB file with your input molecule translated to match the offset used in creating cutout.mtz

Examples

Preparing density for cut_out_density:

Reading in an cut density in map from the command line you can type:

phenix.cut_out_density model.pdb map_file=map.ccp4

Preparing density for molecular replacement in Phaser:

The for. program this document with none of the defaults approximately. You have to provide a PDB file with atoms in the region of interest and a map file covering the region of interest. The program will cut out the density in the region of the PDB file and write out a new map file. The output coordinates are shifted to be consistent with the original coordinates in the input PDB file.

phenix.cut_out_density for_phaser=true model.pdb=1ubq.pdb map_file=1ubq.ccp4

List of all available keywords

```
cut_out_density
  model = None
    Input PDB file defining region to cut out
  map_file = None
    Input EXTC file with map coefficients
  map_coeffs_file = None
    Input EXTC file with map coefficients
    If map_coeffs_file and map_file are both specified, the
    map_coeffs will be used to calculate a new map, then the
    new map will be used to calculate new map coefficients.
    Normally specify either map_file or map_coeffs_file.
    Normally specify only one of map_file and map_coeffs_file.
  pdb_for_center = None
    PDB file defining a point to be the center of the region
    to be cut out. The center of the region will be the
    centroid of the selected atoms in this file.
    If pdb_for_center and pdb_for_region are both specified,
    the center will be the centroid of the selected atoms in
    pdb_for_center and the region will be defined by the input
    pdb_for_region and radius_from_pdb_for_region.
  pdb_for_region = None
    PDB file defining a region to be cut out. The region will
    be defined by all points within a specified distance of
    points in this file.
    If pdb_for_center and pdb_for_region are both specified,
    the center will be the centroid of the selected atoms in
    pdb_for_center and the region will be defined by the input
    pdb_for_region and radius_from_pdb_for_region.
  radius_from_pdb_for_region = None
    Radius around points in pdb_for_region to be cut out.
    If radius_from_pdb_for_region is specified, the region
    will be defined by all points within a specified distance
    of points in pdb_for_region.
  selection_for_center = None
    Selection string for selecting atoms to be used to define
    the center of the region to be cut out.
    Example: selection_for_center="chain A and ca"
    If selection_for_center and pdb_for_center are both
    specified, the center will be the centroid of the selected
    atoms in pdb_for_center.
  selection_for_region = None
    Selection string for selecting atoms to be used to define
    the region to be cut out.
    Example: selection_for_region="chain A and ca"
    If selection_for_region and pdb_for_region are both
    specified, the region will be defined by the selected
    atoms in pdb_for_region and radius_from_pdb_for_region.
  radius_from_pdb_for_region = None
    Radius around points in pdb_for_region to be cut out.
    If radius_from_pdb_for_region is specified, the region
    will be defined by all points within a specified distance
    of points in pdb_for_region.
  output_file_root = None
    Root for output files
  shift_to_original_coordinates = True
    Shift output coordinates to be consistent with original
    coordinates in input EXTC file (unless cut out coordinates
    are specified).
  cut_out_coordinates = None
    Cut out coordinates (in Angstroms) to be used to define the
    region to be cut out. Specify six numbers: xmin,xmax,
    ymin,ymax,zmin,zmax
  cut_out_unit_cell_and_space_group = False
    Cut out the unit cell and space group coordinates that are
    in the specified region of the unit cell.
  cut_out_density = True
    Cut out density in the specified region
  shift_to_center = False
    Shift the center of the region to be cut out to the origin
  shift_vector = None
    Shift vector to be applied to the coordinates
  shift_by_pdb_center = None
    Shift the center of the region to be cut out to the center
    of the selected atoms in this PDB file.
  shift_by_selection_center = None
    Shift the center of the region to be cut out to the center
    of the selected atoms in the input PDB file.
  shift_by_cell_center = None
    Shift the center of the region to be cut out to the center
    of the unit cell.
  shift_to_zero = False
    Shift the center of the region to be cut out to the origin
  shift_to_zero_if_positive = None
    Shift the center of the region to be cut out to the origin
    if all coordinates are positive.
  shift_to_zero_if_negative = None
    Shift the center of the region to be cut out to the origin
    if all coordinates are negative.
  shift_to_zero_if_specified = None
    Shift the center of the region to be cut out to the origin
    if any coordinates are specified.
  shift_to_zero_if_not_specified = None
    Shift the center of the region to be cut out to the origin
    if any coordinates are not specified.
  shift_to_zero_if_all_specified = None
    Shift the center of the region to be cut out to the origin
    if all coordinates are specified.
  shift_to_zero_if_any_specified = None
    Shift the center of the region to be cut out to the origin
    if any coordinates are specified.
  radius = None
    Radius of region to be cut out
  radius_from_pdb_for_region = None
    Radius around points in pdb_for_region to be cut out.
    If radius_from_pdb_for_region is specified, the region
    will be defined by all points within a specified distance
    of points in pdb_for_region.
  radius_from_pdb_for_center = None
    Radius around points in pdb_for_center to be cut out.
    If radius_from_pdb_for_center is specified, the region
    will be defined by all points within a specified distance
    of points in pdb_for_center.
  xmin = None
    Minimum x to be cut out
  xmax = None
    Maximum x to be cut out
  ymin = None
    Minimum y to be cut out
  ymax = None
    Maximum y to be cut out
  zmin = None
    Minimum z to be cut out
  zmax = None
    Maximum z to be cut out
  resolution = None
    Resolution to be used in calculating new map coefficients
  shift_cutout = True
    Shift cutout to be consistent with original coordinates
  write_cutout_pdb = True
    Write out cutout PDB file
  write_cutout_mtz = True
    Write out cutout MTZ file
  write_cutout_ccp4 = True
    Write out cutout CCP4 file
  write_cutout_xplor = False
    Write out cutout XPLOR file
  write_cutout_shelx = False
    Write out cutout SHELX file
  write_cutout_phenix = False
    Write out cutout PHENIX file
  write_cutout_all = False
    Write out all cutout files
  write_cutout_any = False
    Write out any cutout files
  write_cutout_none = False
    Write out no cutout files
  for_phaser = False
    Prepare for Phaser
  for_molecular_replacement = False
    Prepare for molecular replacement
  verbose = False
    Verbose output
  debug = False
    Debug output
```

```
    cutoff_day_title_name = None    # Title name for day title of cutoff_as_weekfirst
    cutoff_day_title_length = None  # Max length for day title of cutoff_as_weekfirst
    cutoff_day_title_index = None   # Index for header field of cutoff_as_weekfirst
    cutoff_day_title_separator = '' # Separator between day titles of cutoff_as_weekfirst
structure:
    separator = ''                  # Separator structures among fields with the be printed
    max_printed_str = None
cutoff_tagged:
    high_resolution = None          # Resolution of cutoff tagged mode (cutoff_tagged=True) with
                                    # high-resolution. Set the cutoff to minutes if this is
                                    # False (default).
    high_resolution_point = 0.00    # Separator of decimal seconds when high-resolution
                                    # (high_resolution=True). Set the cutoff to seconds if
    cutoff_point = None             # Cutoff point of cutoff tagged mode (cutoff_tagged=True).
                                    # Specify the cutoff point as the decimal seconds since the
                                    # beginning of the day. Set the cutoff to midnight if
                                    # cutoff_point=0.0. Set the cutoff to noon if
                                    # cutoff_point=43200.0.
    cutoff_fix_position = False     # Specify if the cutoff position fixed or not (cutoff
                                    # tagged=True). If set to True, the cutoff position is fixed
                                    # to the specified cutoff point (cutoff_point). If set to
                                    # False, the cutoff point is calculated from the specified
                                    # cutoff point (cutoff_point) and the current time. For
                                    # example, if cutoff_point=43200.0 (noon) and
                                    # cutoff_fix_position=False, the cutoff point is noon of
                                    # today if the current time is before noon, and noon of
                                    # tomorrow if the current time is after noon.
    cutoff_presentation = None      # Cutoff presentation mode (cutoff tagged=True). Set cutoff
                                    # to the specified cutoff point (cutoff_point) if
                                    # cutoff_presentation=True. Set cutoff to the current time if
                                    # cutoff_presentation=False. Set cutoff to the current time
                                    # if cutoff_presentation=None and the current time is after
                                    # the cutoff point (cutoff_point). Set cutoff to the cutoff
                                    # point (cutoff_point) if cutoff_presentation=None and the
                                    # current time is before the cutoff point (cutoff_point).
    day_point = None                # Cutoff point of the first cutoff day (cutoff tagged=True).
                                    # Specify the cutoff point as the decimal seconds since the
                                    # beginning of the day. Set the cutoff to midnight if
    padding = 1                     # Padding of cutoff tagged mode (cutoff tagged=True). Set
                                    # cutoff to the specified cutoff point (cutoff_point) if
                                    # cutoff_presentation=True. Set cutoff to the current time if
                                    # cutoff_presentation=False. Set cutoff to the current time
                                    # if cutoff_presentation=None and the current time is after
                                    # the cutoff point (cutoff_point). Set cutoff to the cutoff
                                    # point (cutoff_point) if cutoff_presentation=None and the
                                    # current time is before the cutoff point (cutoff_point).
    cutoff_type = 'day' (enum)      # Cutoff type of cutoff tagged mode (cutoff tagged=True).
                                    # Specify the cutoff type. Set the cutoff to the
                                    # beginning of the current day if cutoff_type='day'. Set
                                    # the cutoff to the beginning of the current week if
                                    # cutoff_type='week'. Set the cutoff to the beginning of the
                                    # current month if cutoff_type='month'. Set the cutoff to
                                    # the beginning of the current year if cutoff_type='year'.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # year if cutoff_type='fiscal_year'. Set the cutoff to the
                                    # beginning of the current fiscal quarter if
                                    # cutoff_type='fiscal_quarter'. Set the cutoff to the
                                    # beginning of the current fiscal month if
                                    # cutoff_type='fiscal_month'. Set the cutoff to the
                                    # beginning of the current fiscal week if
                                    # cutoff_type='fiscal_week'. Set the cutoff to the
                                    # beginning of the current fiscal day if
                                    # cutoff_type='fiscal_day'. Set the cutoff to the
                                    # beginning of the current fiscal hour if
                                    # cutoff_type='fiscal_hour'. Set the cutoff to the
                                    # beginning of the current fiscal minute if
                                    # cutoff_type='fiscal_minute'. Set the cutoff to the
                                    # beginning of the current fiscal second if
                                    # cutoff_type='fiscal_second'. Set the cutoff to the
                                    # beginning of the current fiscal millisecond if
                                    # cutoff_type='fiscal_millisecond'. Set the cutoff to the
                                    # beginning of the current fiscal microsecond if
                                    # cutoff_type='fiscal_microsecond'. Set the cutoff to the
                                    # beginning of the current fiscal nanosecond if
                                    # cutoff_type='fiscal_nanosecond'. Set the cutoff to the
    cutoff_weekday_option = 'Mo'    # Weekday option of cutoff tagged mode (cutoff tagged=True).
                                    # Specify the cutoff weekday. Set the cutoff to the
    cutoff_week = False             # Week option of cutoff tagged mode (cutoff tagged=True).
                                    # Specify the cutoff week. Set the cutoff to the
                                    # beginning of the current week if cutoff_week=False. Set
                                    # the cutoff to the beginning of the next week if
                                    # cutoff_week=True. Set the cutoff to the beginning of the
                                    # current week if cutoff_week=None and the current time is
                                    # after the cutoff point (cutoff_point). Set the cutoff to
                                    # the beginning of the next week if cutoff_week=None and the
                                    # current time is before the cutoff point (cutoff_point).
    cutoff_weekfirst_option = 'Mo'  # Weekfirst option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff weekfirst. Set the
    cutoff_month = False            # Month option of cutoff tagged mode (cutoff tagged=True).
                                    # Specify the cutoff month. Set the cutoff to the
                                    # beginning of the current month if cutoff_month=False.
                                    # Set the cutoff to the beginning of the next month
                                    # if cutoff_month=True. Set the cutoff to the beginning of
                                    # the current month if cutoff_month=None and the current
                                    # time is after the cutoff point (cutoff_point). Set the
                                    # cutoff to the beginning of the next month if
                                    # cutoff_month=None and the current time is before the
                                    # cutoff point (cutoff_point).
    cutoff_quarter = False          # Quarter option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff quarter. Set the
    cutoff_year = False             # Year option of cutoff tagged mode (cutoff tagged=True).
                                    # Specify the cutoff year. Set the cutoff to the
                                    # beginning of the current year if cutoff_year=False.
                                    # Set the cutoff to the beginning of the next year
                                    # if cutoff_year=True. Set the cutoff to the beginning of
                                    # the current year if cutoff_year=None and the current
                                    # time is after the cutoff point (cutoff_point). Set the
                                    # cutoff to the beginning of the next year if
                                    # cutoff_year=None and the current time is before the
                                    # cutoff point (cutoff_point).
    cutoff_fiscal_year = None       # Fiscal year option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal year. Set the
    cutoff_fiscal_quarter = None    # Fiscal quarter option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal quarter. Set the
    cutoff_fiscal_month = None      # Fiscal month option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal month. Set the
    cutoff_fiscal_week = None       # Fiscal week option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal week. Set the
    cutoff_fiscal_day = None        # Fiscal day option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal day. Set the
    cutoff_fiscal_hour = None       # Fiscal hour option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal hour. Set the
    cutoff_fiscal_minute = None     # Fiscal minute option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal minute. Set the
    cutoff_fiscal_second = None     # Fiscal second option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal second. Set the
    cutoff_fiscal_millisecond = None # Fiscal millisecond option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal millisecond. Set
    cutoff_fiscal_microsecond = None # Fiscal microsecond option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal microsecond. Set
    cutoff_fiscal_nanosecond = None # Fiscal nanosecond option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal nanosecond. Set
    cutoff_fiscal_weekfirst = None  # Fiscal weekfirst option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal weekfirst. Set
    cutoff_fiscal_weekfirst_option = None # Fiscal weekfirst option of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal weekfirst. Set
    cutoff_fiscal_month_type = None 4-5-4 fiscal month type of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff 4-5-4 fiscal month type.
                                    # Set the cutoff to the beginning of the current 4-5-4
                                    # fiscal month if cutoff_fiscal_month_type='4-5-4'. Set
                                    # the cutoff to the beginning of the next 4-5-4 fiscal
                                    # month if cutoff_fiscal_month_type='4-5-4'. Set the
                                    # cutoff to the beginning of the current fiscal month
                                    # if cutoff_fiscal_month_type='fiscal'. Set the cutoff
                                    # to the beginning of the next fiscal month
                                    # if cutoff_fiscal_month_type='fiscal'.
    cutoff_fiscal_week_type = None  # Fiscal week type of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal week type. Set
                                    # the cutoff to the beginning of the current fiscal week
                                    # if cutoff_fiscal_week_type='fiscal'. Set the cutoff
                                    # to the beginning of the next fiscal week
                                    # if cutoff_fiscal_week_type='fiscal'.
    cutoff_fiscal_week_index = None 1-53 fiscal week index of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff 1-53 fiscal week index.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # week if cutoff_fiscal_week_index=None. Set the cutoff
                                    # to the beginning of the next fiscal week
                                    # if cutoff_fiscal_week_index=None.
    cutoff_fiscal_week_index_type = None # Fiscal week index type of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal week index type.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # week if cutoff_fiscal_week_index_type='fiscal'. Set
                                    # the cutoff to the beginning of the next fiscal week
                                    # if cutoff_fiscal_week_index_type='fiscal'.
    cutoff_fiscal_day_index = None  # Fiscal day index of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal day index.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # day if cutoff_fiscal_day_index=None. Set the cutoff
                                    # to the beginning of the next fiscal day
                                    # if cutoff_fiscal_day_index=None.
    cutoff_fiscal_day_index_type = None # Fiscal day index type of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal day index type.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # day if cutoff_fiscal_day_index_type='fiscal'. Set
                                    # the cutoff to the beginning of the next fiscal day
                                    # if cutoff_fiscal_day_index_type='fiscal'.
    cutoff_fiscal_hour_index = None 0-23 fiscal hour index of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal hour index.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # hour if cutoff_fiscal_hour_index=None. Set the cutoff
                                    # to the beginning of the next fiscal hour
                                    # if cutoff_fiscal_hour_index=None.
    cutoff_fiscal_hour_index_type = None # Fiscal hour index type of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal hour index type.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # hour if cutoff_fiscal_hour_index_type='fiscal'. Set
                                    # the cutoff to the beginning of the next fiscal hour
                                    # if cutoff_fiscal_hour_index_type='fiscal'.
    cutoff_fiscal_minute_index = None # Fiscal minute index of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal minute index.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # minute if cutoff_fiscal_minute_index=None. Set the
                                    # cutoff to the beginning of the next fiscal minute
                                    # if cutoff_fiscal_minute_index=None.
    cutoff_fiscal_minute_index_type = None # Fiscal minute index type of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal minute index type.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # minute if cutoff_fiscal_minute_index_type='fiscal'.
                                    # Set the cutoff to the beginning of the next fiscal
                                    # minute if cutoff_fiscal_minute_index_type='fiscal'.
    cutoff_fiscal_second_index = None # Fiscal second index of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal second index.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # second if cutoff_fiscal_second_index=None. Set the
                                    # cutoff to the beginning of the next fiscal second
                                    # if cutoff_fiscal_second_index=None.
    cutoff_fiscal_second_index_type = None # Fiscal second index type of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal second index type.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # second if cutoff_fiscal_second_index_type='fiscal'.
                                    # Set the cutoff to the beginning of the next fiscal
                                    # second if cutoff_fiscal_second_index_type='fiscal'.
    cutoff_fiscal_millisecond_index = None # Fiscal millisecond index of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal millisecond index.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # millisecond if cutoff_fiscal_millisecond_index=None.
                                    # Set the cutoff to the beginning of the next fiscal
                                    # millisecond if cutoff_fiscal_millisecond_index=None.
    cutoff_fiscal_millisecond_index_type = None # Fiscal millisecond index type of cutoff tagged mode
                                    # (cutoff tagged=True). Specify the cutoff fiscal
                                    # millisecond index type. Set the cutoff to the beginning
                                    # of the current fiscal millisecond if
                                    # cutoff_fiscal_millisecond_index_type='fiscal'. Set
                                    # the cutoff to the beginning of the next fiscal
                                    # millisecond if cutoff_fiscal_millisecond_index_type='fiscal'.
    cutoff_fiscal_microsecond_index = None # Fiscal microsecond index of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal microsecond index.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # microsecond if cutoff_fiscal_microsecond_index=None.
                                    # Set the cutoff to the beginning of the next fiscal
                                    # microsecond if cutoff_fiscal_microsecond_index=None.
    cutoff_fiscal_microsecond_index_type = None # Fiscal microsecond index type of cutoff tagged mode
                                    # (cutoff tagged=True). Specify the cutoff fiscal
                                    # microsecond index type. Set the cutoff to the beginning
                                    # of the current fiscal microsecond if
                                    # cutoff_fiscal_microsecond_index_type='fiscal'. Set
                                    # the cutoff to the beginning of the next fiscal
                                    # microsecond if cutoff_fiscal_microsecond_index_type='fiscal'.
    cutoff_fiscal_nanosecond_index = None # Fiscal nanosecond index of cutoff tagged mode (cutoff
                                    # tagged=True). Specify the cutoff fiscal nanosecond index.
                                    # Set the cutoff to the beginning of the current fiscal
                                    # nanosecond if cutoff_fiscal_nanosecond_index=None.
                                    # Set the cutoff to the beginning of the next fiscal
                                    # nanosecond if cutoff_fiscal_nanosecond_index=None.
    cutoff_fiscal_nanosecond_index_type = None # Fiscal nanosecond index type of cutoff tagged mode
                                    # (cutoff tagged=True). Specify the cutoff fiscal
                                    # nanosecond index type. Set the cutoff to the beginning
                                    # of the current fiscal nanosecond if
                                    # cutoff_fiscal_nanosecond_index_type='fiscal'. Set
                                    # the cutoff to the beginning of the next fiscal
                                    # nanosecond if cutoff_fiscal_nanosecond_index_type='fiscal'.
```

Phenix *Python-based Hierarchical Rhombohedral for Integrated Kaleidoscopy*

Visualizing reflection data in Phenix

Contents

- Overview
- 3D viewer
- 2D viewer
- 1D viewer

Overview

The rhombohedral solution space viewer is used to examine data in hexagonal space, as a diagnostic and learning tool. Although rhombohedral solution space is a mathematically convenient way to represent the space of possible lattices, it is difficult to visualize and interpret in 3D. Alternatively, rhombohedral solution space can be visualized in the form of slices, such as a 3D view of projected reflections, or "episcopic-precession-photographs". These are largely analogous to the familiar precession photographs produced by the program Mosflm.

phenix.data_viewer uses the libraries/tools from the CCP4 suite "Reflection tools". Unlike the 3D and 2D versions, which are based on the Phenix GUI, the 1D version is a standalone tool. It is intended for quick inspection of reflection data, and needs a reasonable field graphics card to be responsive for the 3D graphics. For this reason, we do not recommend running phenix.data_viewer on remote machines, unless the connection is very fast and the remote machine has a good graphics card. The 3D and 2D versions are intended for interactive use, and are not suitable for batch processing. The 1D version is a simple command-line utility, and can be used in batch mode. It is also more suitable than the other two versions for remote use, and is suitable for slow or low-bandwidth connections.

3D viewer

By slicing reflections files, this data 3D viewer provides an overview of a dataset, whose lattice is one dimension less than the reciprocal reciprocal. Observations of special special reflections and systematic lattice plane and extinctions indicate, variety of lattice centering, and the presence of twinning, can be easily identified. Although the 3D viewer is based on the Phenix GUI, it requires a fairly fast graphics card and recent version of OpenGL (version 2.0 or higher).

Phenix
Data Viewer
Data Source
Reflection File
/home/pjanson/Phenix/Data/Reflections/1ubq.mtz
Data Type
Reflection Data
Data Array
FOBS,SIGFOBS
Data Array
FOBS,SIGFOBS
Data Array
FOBS,SIGFOBS

In this case the space group is 18 with anomalous data, so the symmetry unique reflections fill two 3D shapes (Friedel mates) which are related by inversion symmetry. Because the data are anomalous, the two shapes are not exactly equal, but the underlying mechanism of reciprocal-space symmetry still applies. Crucially, the two shapes are related by inversion symmetry, so the same reflections appear in both shapes. Because the data are anomalous, the two shapes are not identical, but the underlying mechanism of reciprocal-space symmetry still applies. Crucially, the two shapes are related by inversion symmetry, so the same reflections appear in both shapes.

The slider can be manipulated with the controls on the left-hand side of the viewer, this moves the slicer to change the symmetry or provide anomalous data if one is present in the input file. A particularly useful option is the ability to change the slicer to show the Friedel mates (anomalous data).

Most datasets will have at least a handful of times at high resolution, and often the underlying spacegroup, reflections and data be absent due to resonance overlap. In this case a large contiguous region of missing data is visible, the slicer can be used to see the underlying reflections and understand why the data are missing. In this case the reflections are missing because the underlying symmetry forces a particular structure of reciprocal space. Because the underlying symmetry forces a particular structure of reciprocal space, the reflections are missing because the underlying symmetry forces a particular structure of reciprocal space and reciprocal space is constrained at various degree of refinement, especially if large regions of reciprocal space are systematically absent.

2D viewer

The 2D view handles symmetry unique data differently from the 3D version. It will always expand these data to the full reciprocal space, this means that the slicer will show the symmetry related reflections in the reciprocal space regardless of the input file (all or asymmetric). This will result in a view something like this (here using the mtzdump example).

In this example both missing reflections (small white spots) and systematic absences (large purple spot) are visible. Because the underlying symmetry forces a particular structure of reciprocal space, both missing reflections and systematic absences are displayed instead of interpolating, and quite obviously the data are probably not centrified or processed in the expected reciprocal space symmetry for this crystal.

Phenix *Python-based Hierarchical Environment for Integrated Nallography*

phenix.dxn_refine: DEN refinement in Phenix

Deformable elastic network (DEN) refinement is a refinement protocol that uses a global elastic network to maintain local bond geometry while preserving the large global domain motions over the course of several thousand steps of molecular dynamics.

The DEN restraint network is a set of elastic attractive harmonic restraints between atoms 3 to 5 Angstroms apart and is generated from the starting model. The DEN restraints are then held fixed for the duration of the refinement. The corresponding distances in a reference model (such as a higher resolution structure or homology model) or for a set of randomly displaced atoms are also stored. The DEN restraints are then used in a molecular dynamics simulation to drive the structure of interest toward the reference state. DEN restraints have been known to be beneficial in refinement of structures at low resolution.

DEN was originally described by Brunger and colleagues in

Deformable elastic network refinement. Acta Crystallogr D Biol Crystallogr. 2007 Jan; 63(Pt 1):29-39. Epub 2006 Nov 28. PubMed PMID: 17164527 **Scale-variation biomolecular crystallography with low-resolution data.** Acta Cryst D. 2010 Jan 1; 66(Pt 1): 12-21. PMCID: PMC2803147

Optimization

The speed of the DEN restraint network is controlled by two variable parameters, gamma, which controls the number of nonbonded interactions and thus the speed of the calculation, and the number of nonbonded interactions to the overall refinement energy term (see the above references for details). To get the most out of a DEN refinement, one must find the optimal values for these parameters. Unfortunately, the optimal values for gamma are very rare instances, and is best carried out on a machine with many processors.

The DEN refinement protocol has been implemented in the Phenix software package, using the OpenMM library (v. 4.1.1, 6.0.1, 6.0.1b, 6.0.1c, 6.0.1d, 6.0.1e) and tested on a wide variety of a machine to find the optimum value. The optimum value for gamma is then used in a production refinement by the main macro-parameter, by setting macro-cycles=20 and run the optimization step on 20 processors.

Using DEN

To use the DEN refinement the version:

1. Develop dxn-refine-mpi.zip data into dxnrefine-mpi

See the full list of options below

There is also a DEN refinement GUI for those who prefer a graphical interface.

phenix.dxn_refine uses a modified version of the default phenix.refine parameters optimized for DEN refinement.

The DEN-specific subset of refinement parameters:

```
refinement {
  dxn {
    enabled = True
    dxn {
      gamma = 1.7976931348623157e+308
      nonbonded_cutoff = 1.7976931348623157e+308
      nonbonded_switch = 1.7976931348623157e+308
    }
    dxn {
      dxn_weight_initial = None
      dxn_weight = 0.5
      dxn_weight = 0.5
      dxn_weight = 0.5
      dxn_weight = 0.5
      dxn_weight_initial = 0.5 0.5 0.5 0.5
      dxn_weight_initial = 0.5 0.5 0.5 0.5
      temperature = 300.0
      temperature_initial = 300.0
      temperature_initial = 300.0 0.0 0.0
      dxn_cutoff = 5.0
      dxn_cutoff_initial = 5.0
      dxn_cutoff_initial = 5.0 5.0 5.0
      dxn_cutoff = 5.0
      dynamics_method = velocity verlet
      dynamics_method = leap frog
      dynamics_method = verlet
      integrator_type = 0
      integrator_type = 0 0 0 0
      integrator_type = 0 0 0 0
      integrator_type = 0 0 0 0
      integrator_type = 0 0 0 0
      dynamics_steps = 0
      dynamics_steps = 0 0 0 0
      dynamics_steps = 0 0 0 0
      dynamics_steps = 0 0 0 0
      dynamics_steps = 0 0 0 0
    }
    dxn_cutoff_initial = 5.0
    dxn_cutoff_initial = 5.0
    dxn_cutoff = 5.0
    dxn_cutoff = 5.0
    dynamics_method = velocity verlet
    dynamics_method = velocity verlet
    dynamics_method = velocity verlet
    dynamics_method = velocity verlet
    dynamics_method = velocity verlet
    dynamics_steps = 0
    dynamics_steps = 0
    dynamics_steps = 0
```

PHENIX *Python based Hierarchical Environment for Integrated Xtallography*

Density modification with with phenix.density_modification

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- Run specifying NCS operators
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- Literature
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- List of all available keywords
- List of all available keywords

Author(s)

- phenix.density_modification: Tom Terwilliger

Purpose

phenix.density_modification is a tool to run Resolve to carry out density modification, including the use of NCS operators and phase information. Phases may be provided in terms of phases and figure of merit, or in terms of Hendrickson-Lattman coefficients. Output may be in terms of phases or Hendrickson-Lattman coefficients.

Usages

How phenix.density_modification works

In phenix.density_modification phases are expressed in combining any existing phase information with phase information from density modification. Hendrickson-Lattman coefficients are used to express the phase information in density modification and in combining it with any existing phase information. The applications, in order of complexity, are:

- A fully solved model
- Density modification with NCS
- Density modification without NCS
- Density modification starting with phases and HL coefficients

Density modification starting with phases and HL coefficients

This kind of density modification is normally carried out after experimental phasing, but it can also be carried out with any phase information. Phases and HL coefficients are used.

In these cases you have phases and phase probability information (2 SIGN AND FOM, HLA HLB HLC HLD).

When to density modification, the amplitudes (F SIGF) are normally constructed by amplitude expansion. The phases are combined with any existing phase information by combining the Hendrickson-Lattman coefficients. The phases are then expanded into a set of phase probabilities (HLA HLB HLC HLD) and the amplitudes are constructed from the phases and the expanded HL coefficients.

A starting map is calculated from 2 FOBS FOM. The squares of the macromolecule and solvent are estimated in reciprocal space using the FOM and the phases, and a starting map is calculated. This starting map is then transformed back into HL coefficients and is used as a map mask for a new density modification.

Phases are expressed in terms with the HL coefficients and is used a map mask for a new density modification. The phases are combined with the HL coefficients and

Density modification with NCS

If one supplies NCS operators, phenix.density_modification will automatically figure out the region over which the NCS operators are to be applied and will carry out NCS averaging in density modification. The NCS operators are specified in the input parameter file, or in a separate NCS file, in a well-defined format. The formats of NCS files are described in the Resolve documentation.

Density modification with a model

If one supplies a model, phenix.density_modification assumes a solved model. Then the data are corrected for shrinkage on the basis of the model, and the phases of the model are used to calculate a map. Then density modification is carried out and the corrected phases for experimental phasing. There is first step in carried out in which model density is subtracted from the map before density modification.

To minimize bias in coefficients from high-phase and low-phase cycle phases, phase probabilities, four Hendrickson-Lattman coefficients, and figure of merit are used. Phases are chosen, and FOM with short model bias and bias in off-diagonal coefficients are

Note on R-values in density modification

The R-value for density modification is quite different from a refinement R. Basically the statistical (maximum likelihood) R-factor is calculated between the observed structure factor amplitudes and the structure factor amplitudes calculated from the current model. In density modification, the structure factor amplitudes are not calculated from a model, but are "filled" from phase information. Thus the R-factor between the observed and the calculated will be very high. The R-factor between the observed and the calculated will be very low. The

Phenic — *Python-based Hierarchical Movement for Enzymatic Kinetics*

Merging two models with density_outside_model

Author(s)

- Alexis Jacquier, Leopold Tom Stockinger

Purpose

This function takes a model and map coefficients and returns new map coefficients with density set to zero near the model.

Usage

The main use of phenic.density_outside_model are:

- Creating a map where all the parts of the map that have been explained by a model are removed.

How density_outside_model works:

Density_outside_model calculates a new field that map coefficients. Then all map values at points near an atom are multiplied by a factor. This factor is 0 at the atom and increases to 1 at a specified distance.

Especially the model can be trimmed so that the rest is 100% meaningful or each segment of the model are not too close.

Output files from density_outside_model

density_outside_model. (.mtz) the new map with the coefficients.

Examples

Standard use of density_outside_model:

Running density_outside_model is easy.Then the command line also can hyper:

```
phenic density_outside_model -pdb=model.pdb -mtz=input.mtz
phenic density_outside_model -h
```

Possible Problems

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
density_outside_model
    input_files
        pdb_file : None                 Input PDB file matching region to remove from map
        mtz_in : None                   Input MTZ file with map coefficients
        mtz_out : density_outside.mtz   Output MTZ file with map coefficients. Contains the input map with
                                        zero, and optionally the specified region. Phenic expects
                                        the input map to be normalized. Phenic will output the
                                        coefficients as they are in the input file. Use
                                        phenic.normalize_map_coefficients to normalize the map
                                        before or after using this tool.
    output_files
        log : density_removed.log       Output log file
        pdb_out : density_removed.pdb   Output PDB file
    density_parameters
        radius : 2.0                    Radius (A) within which to zero out density_removed
        fade_out : True,False           Optional temporary with discontinuity
        fade_out_dist : 1.0             Output distance where fade_out is to be active
    density_removed_region
        density_removed_model_radius    : 0.0,1.0,inf,[0.0,1.0,inf,...]
                                        Radius around atoms in model. Map coefficients within
                                        this radius are set to zero. Optionally, a second value
                                        can be specified for a different radius for atoms matching
                                        the atom type of the corresponding atom selection specified
                                        in the next keyword.
        include_atoms : [,]             Atoms to include in model. Map coefficients within
                                        density_removed_model_radius of these atoms are set to zero.
        atom_selection : None           Optional atom selection. Only atoms matching the atom selection
                                        are used as centers for density_removed_model_radius.
                                        Default: all atoms. Supports all PHENIX atom selection
                                        syntax.
        density_removed_mode            : 0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144,145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,180,181,182,183,184,185,186,187,188,189,190,191,192,193,194,195,196,197,198,199,200,201,202,203,204,205,206,207,208,209,210,211,212,213,214,215,216,217,218,219,220,221,222,223,224,225,226,227,228,229,230,231,232,233,234,235,236,237,238,239,240,241,242,243,244,245,246,247,248,249,250,251,252,253,254,255,256,257,258,259,260,261,262,263,264,265,266,267,268,269,270,271,272,273,274,275,276,277,278,279,280,281,282,283,284,285,286,287,288,289,290,291,292,293,294,295,296,297,298,299,300,301,302,303,304,305,306,307,308,309,310,311,312,313,314,315,316,317,318,319,320,321,322,323,324,325,326,327,328,329,330,331,332,333,334,335,336,337,338,339,340,341,342,343,344,345,346,347,348,349,350,351,352,353,354,355,356,357,358,359,360,361,362,363,364,365,366,367,368,369,370,371,372,373,374,375,376,377,378,379,380,381,382,383,384,385,386,387,388,389,390,391,392,393,394,395,396,397,398,399,400,401,402,403,404,405,406,407,408,409,410,411,412,413,414,415,416,417,418,419,420,421,422,423,424,425,426,427,428,429,430,431,432,433,434,435,436,437,438,439,440,441,442,443,444,445,446,447,448,449,450,451,452,453,454,455,456,457,458,459,460,461,462,463,464,465,466,467,468,469,470,471,472,473,474,475,476,477,478,479,480,481,482,483,484,485,486,487,488,489,490,491,492,493,494,495,496,497,498,499,500,501,502,503,504,505,506,507,508,509,510,511,512,513,514,515,516,517,518,519,520,521,522,523,524,525,526,527,528,529,530,531,532,533,534,535,536,537,538,539,540,541,542,543,544,545,546,547,548,549,550,551,552,553,554,555,556,557,558,559,560,561,562,563,564,565,566,567,568,569,570,571,572,573,574,575,576,577,578,579,580,581,582,583,584,585,586,587,588,589,590,591,592,593,594,595,596,597,598,599,600,601,602,603,604,605,606,607,608,609,610,611,612,613,614,615,616,617,618,619,620,621,622,623,624,625,626,627,628,629,630,631,632,633,634,635,636,637,638,639,640,641,642,643,644,645,646,647,648,649,650,651,652,653,654,655,656,657,658,659,660,661,662,663,664,665,666,667,668,669,670,671,672,673,674,675,676,677,678,679,680,681,682,683,684,685,686,687,688,689,690,691,692,693,694,695,696,697,698,699,700,701,702,703,704,705,706,707,708,709,710,711,712,713,714,715,716,717,718,719,720,721,722,723,724,725,726,727,728,729,730,731,732,733,734,735,736,737,738,739,740,741,742,743,744,745,746,747,748,749,750,751,752,753,754,755,756,757,758,759,760,761,762,763,764,765,766,767,768,769,770,771,772,773,774,775,776,777,778,779,780,781,782,783,784,785,786,787,788,789,790,791,792,793,794,795,796,797,798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000,1001,1002,1003,1004,1005,1006,1007,1008,1009,1010,1011,1012,1013,1014,1015,1016,1017,1018,1019,1020,1021,1022,1023,1024,1025,1026,1027,1028,1029,1030,1031,1032,1033,1034,1035,1036,1037,1038,1039,1040,1041,1042,1043,1044,1045,1046,1047,1048,1049,1050,1051,1052,1053,1054,1055,1056,1057,1058,1059,1060,1061,1062,1063,1064,1065,1066,1067,1068,1069,1070,1071,1072,1073,1074,1075,1076,1077,1078,1079,1080,1081,1082,1083,1084,1085,1086,1087,1088,1089,1090,1091,1092,1093,1094,1095,1096,1097,1098,1099,1100,1101,1102,1103,1104,1105,1106,1107,1108,1109,1110,1111,1112,1113,1114,1115,1116,1117,1118,1119,1120,1121,1122,1123,1124,1125,1126,1127,1128,1129,1130,1131,1132,1133,1134,1135,1136,1137,1138,1139,1140,1141,1142,1143,1144,1145,1146,1147,1148,1149,1150,1151,1152,1153,1154,1155,1156,1157,1158,1159,1160,1161,1162,1163,1164,1165,1166,1167,1168,1169,1170,1171,1172,1173,1174,1175,1176,1177,1178,1179,1180,1181,1182,1183,1184,1185,1186,1187,1188,1189,1190,1191,1192,1193,1194,1195,1196,1197,1198,1199,1200,1201,1202,1203,1204,1205,1206,1207,1208,1209,1210,1211,1212,1213,1214,1215,1216,1217,1218,1219,1220,1221,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4222,4223,4224,4225,4226,4227,4228,4229,4230,4231,4232,4233,4234,4235,4236,4237,4238,4239,4240,4241,4242,4243,4244,4245,4246,4247,4248,4249,4250,4251,4252,4253,4254,4255,4256,4257,4258,4259,4260,4261,4262,4263,4264,4265,4266,4267,4268,4269,4270,4271,4272,4273,4274,4275,4276,4277,4278,4279,4280,4281,4282,4283,4284,4285,4286,4287,4288,4289,4290,4291,4292,4293,4294,4295,4296,4297,4298,4299,4300,4301,4302,4303,4304,4305,4306,4307,4308,4309,4310,4311,4312,4313,4314,4315,4316,4317,4318,4319,4320,4321,4322,4323,4324,4325,4326,4327,4328,4329,4330,4331,4332,4333,4334,4335,4336,4337,4338,4339,4340,4341,4342,4343,4344,4345,4346,4347,4348,4349,4350,4351,4352,4353,4354,4355,4356,4357,4358,4359,4360,4361,4362,4363,4364,4365,4366,4367,4368,4369,4370,4371,4372,4373,4374,4375,4376,4377,4378,4379,4380,4381,4382,4383,4384,4385,4386,4387,4388,4389,4390,4391,4392,4393,4394,4395,4396,4397,4398,4399,4400,4401,4402,4403,4404,4405,4406,4407,4408,4409,4410,4411,4412,4413,4414,4415,4416,4417,4418,4419,4420,4421,4422,4423,4424,4425,4426,4427,4428,4429,4430,4431,4432,4433,4434,4435,4436,4437,4438,4439,4440,4441,4442,4443,4444,4445,4446,4447,4448,4449,4450,4451,4452,4453,4454,4455,4456,4457,4458,4459,4460,4461,4462,4463,4464,4465,4466,4467,4468,4469,4470,4471,4472,4473,4474,4475,4476,4477,4478,4479,4480,4481,4482,4483,4484,4485,4486,4487,4488,4489,4490,4491,4492,4493,4494,4495,4496,4497,4498,4499,4500,4501,4502,4503,4504,4505,4506,4507,4508,4509,4510,4511,4512,4513,4514,4515,4516,4517,4518,4519,4520,4521,4522,4523,4524,4525,4526,4527,4528,4529,4530,4531,4532,4533,4534,4535,4536,4537,4538,4539,4540,4541,4542,4543,4544,4545,4546,4547,4548,4549,4550,4551,4552,4553,4554,4555,4556,4557,4558,4559,4560,4561,4562,4563,4564,4565,4566,4567,4568,4569,4570,4571,4572,4573,4574,4575,4576,4577,4578,4579,4580,4581,4582,4583,4584,4585,4586,4587,4588,4589,4590,4591,4592,4593,4594,4595,4596,4597,4598,4599,4600,4601,4602,4603,4604,4605,4606,4607,4608,4609,4610,4611,4612,4613,4614,4615,4616,4617,4618,4619,4620,4621,4622,4623,4624,4625,4626,4627,4628,4629,4630,4631,4632,4633,4634,4635,4636,4637,4638,4639,4640,4641,4642,4643,4644,4645,4646,4647,4648,4649,4650,4651,4652,4653,4654,4655,4656,4657,4658,4659,4660,4661,4662,4663,4664,4665,4666,4667,4668,4669,4670,4671,4672,4673,4674,4675,4676,4677,4678,4679,4680,4681,4682,4683,4684,4685,4686,4687,4688,4689,4690,4691,4692,4693,4694,4695,4696,4697,4698,4699,4700,4701,4702,4703,4704,4705,4706,4707,4708,4709,4710,4711,4712,4713,4714,4715,4716,4717,4718,4719,4720,4721,4722,4723,4724,4725,4726,4727,4728,4729,4730,4731,4732,4733,4734,4735,4736,4737,4738,4739,4740,4741,4742,4743,4744,4745,4746,4747,4748,4749,4750,4751,4752,4753,4754,4755,4756,4757,4758,4759,4760,4761,4762,4763,4764,4765,4766,4767,4768,4769,4770,4771,4772,4773,4774,4775,4776,4777,4778,4779,4780,4781,4782,4783,4784,4785,4786,4787,4788,4789,4790,4791,4792,4793,4794,4795,4796,4797,4798,4799,4800,4801,4802,4803,4804,4805,4806,4807,4808,4809,4810,4811,4812,4813,4814,4815,4816,4817,4818,4819,4820,4821,4822,4823,4824,4825,4826,4827,4828,4829,4830,4831,4832,4833,4834,4835,4836,4837,4838,4839,4840,4841,4842,4843,4844,4845,4846,4847,4848,4849,4850,4851,4852,4853,4854,4855,4856,4857,4858,4859,4860,4861,4862,4863,4864,4865,4866,4867,4868,4869,4870,4871,4872,4873,4874,4875,4876,4877,4878,4879,4880,4881,4882,4883,4884,4885,4886,4887,4888,4889,4890,4891,4892,4893,4894,4895,4896,4897,4898,4899,4900,4901,4902,4903,4904,4905,4906,4907,4908,4909,4910,4911,4912,4913,4914,4915,4916,4917,4918,4919,4920,4921,4922,4923,4924,4925,4926,4927,4928,4929,4930,4931,4932,4933,4934,4935,4936,4937,4938,4939,4940,4941,4942,4943,4944,4945,4946,4947,4948,4949,4950,4951,4952,4953,4954,4955,4956,4957,4958,4959,4960,4961,4962,4963,4964,4965,4966,4967,4968,4969,4970,4971,4972,4973,4974,4975,4976,4977,4978,4979,4980,4981,4982,4983,4984,4985,4986,4987,4988,4989,4990,4991,4992,4993,4994,4995,4996,4997,4998,4999,5000,5001,5002,5003,5004,5005,5006,5007,5008,5009,5010,5011,5012,5013,5014,5015,5016,5017,5018,5019,5020,5021,5022,5023,5024,5025,5026,5027,5028,5029,5030,5031,5032,5033,5034,5035,5036,5037,5038,5039,5040,5041,5042,5043,5044,5045,5046,5047,5048,5049,5050,5051,5052,5053,5054,5055,5056,5057,5058,5059,5060,5061,5062,5063,5064,5065,5066,5067,5068,5069,5070,5071,5072,5073,5074,5075,5076,5077,5078,5079,5080,5081,5082,5083,5084,5085,5086,5087,5088,5089,5090,5091,5092,5093,5094,5095,5096,5097,5098,5099,5100,5101,5102,5103,5104,5105,5106,5107,5108,5109,5110,5111,5112,5113,5114,5115,5116,5117,5118,5119,5120,5121,5122,5123,5124,5125,5126,5127,5128,5129,5130,5131,5132,5133,5134,5135,5136,5137,5138,5139,5140,5141,5142,5143,5144,5145,5146,5147,5148,5149,5150,5151,5152,5153,5154,5155,5156,5157,5158,5159,5160,5161,5162,5163,5164,5165,5166,5167,5168,5169,5170,5171,5172,5173,5174,5175,5176,5177,5178,5179,5180,5181,5182,5183,5184,5185,5186,5187,5188,5189,5190,5191,5192,5193,5194,5195,5196,5197,5198,5199,5200,5201,5202,5203,5204,5205,5206,5207,5208,5209,5210,5211,5212,5213,5214,5215,5216,5217,5218,5219,5220,5221,5222,5223,5224,5225,5226,5227,5228,5229,5230,5231,5232,5233,5234,5235,5236,5237,5238,5239,5240,5241,5242,5243,5244,5245,5246,5247,5248,5249,5250,5251,5252,5253,5254,5255,5256,5257,5258,5259,5260,5261,5262,5263,5264,5265,5266,5267,5268,5269,5270,5271,5272,5273,5274,5275,5276,5277,5278,5279,5280,5281,5282,5283,5284,5285,5286,5287,5288,5289,5290,5291,5292,5293,5294,5295,5296,5297,5298,5299
```

dock_and_rebuild

Phenix

Python-based Hierarchical Environment for Synchrotron Enhancements

Processing, docking and rebuilding AlphaFold2 and other predicted models in cryo-EM maps

Author(s)

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Purpose

Dock and rebuild combines the functions of processing, docking and rebuilding predicted models produced by AlphaFold, RoseTTAFold and other prediction programs into a single step.

The command line command for dock_and_rebuild is phenix. There are three ways to specify an alphanumeric or other predicted model with a cryo-EM density.

1. Specify a PDB file with predicted models and a density file with the corresponding resolution in the predicted model that should be docked and rebuilt, and specify a chain ID and a residue range.
2. Specify a predicted model and the density file.
3. Specify a predicted model and the density file and a predicted model into the map, keeping placeholder connectors. This is done with phenix.dock_predicted_model.

The third way is for simulated map protein-protein docks into density and then to rebuild all the parts of the predicted model that fit in the density.

How dock_and_rebuild works

The dock_and_rebuild procedure is used as a step in a series of three steps in processing, docking and rebuilding a predicted model in a cryo-EM density. The three steps are: (1) processing the predicted model, (2) docking the processed model into the density, and (3) rebuilding the docked model. Each step can be used by itself or combined with previous steps. The three steps are described below.

The model result for dock_predicted_model is a cryo-sharpening predicted model file (i.e., an AlphaFold model).

The dock result for dock_predicted_model is normally a pdb or mmcif file containing docked models and the map. If the docking is done with placeholder connectors, the result is a pdb file with placeholders.

If you are able to select your chain, keeping only the part representing the chain where the model belongs, that will improve the speed and accuracy of the docking and rebuilding. If you are using the AlphaFold database, you can choose to download only the parts of proteins that fit into the density. If you have AlphaFold output for a complete protein and want to use just a piece of it, you can use phenix.pdbtools to select the part you want to use.

The three steps described above are then carried out, processing the model to obtain domains representing the chains, docking the processed domains into the density, and rebuilding the docked domains. The command phenix.dock_and_rebuild_multiple carries out processing and rebuilding with the predicted model to used a docked version of the model.

Examples

Standard use of dock_and_rebuild:

Running dock_and_rebuild is easy. From the command line you can type:

```
phenix.dock_and_rebuild model.pdb map.mrc
resolution=3.0 chain=A
```

This will carry out all the steps of processing, docking and rebuilding to yield rb_model.pdb

Possible Problems

If your map has already symmetry, this is problematic you might need to run one subunit or try with specify-ncs-type=cyclic (default search is dihedral).

If your model has many domains, it may be better to run processing separately, dock each domain, rebuild it and then dock and rebuild the full model. If you have several copies of the same domain, run AlphaFold with multimer mode to get the relative positions of the domains, then run dock_and_rebuild_multiple. If you have a chain, and want to cut out an exon and dock and rebuild everything from the beginning.

Specific Limitations and problems:

Literature

Additional information

List of all available keywords

```
phenix.dock
  model=pdb file name
  map=ccp4 file name
  ncs_file_name=ncs file name
  ncs_type=ncs type
  chain_id=chain id
  resolution=resolution
  search_radius=search radius
  density_sigma=1.0 float
  density_cutoff=0.0 float
  ncs_copies=ncs copies
  ncs_center=ncs center
  n_fine_fits=n fine fits
  n_coarse_fits=n coarse fits
  max_fit=0.0 float
  max_clash=0.0 float
  search_model_is_ensemble=
  search_ensemble_is_ensemble=
  ensemble_sigma=1.0 float
  ensemble_cutoff=0.0 float
  ensemble_search_radius=
  model_copies=1 int
  search_copies=1 int
  ensemble_search_copies=1 int
  ensemble_model_copies=1 int
  model_center=model center
  search_center=search center
  ensemble_search_center=
  ensemble_model_center=
  model_radius=model radius
  search_radius=search radius
  ensemble_search_radius=
  ensemble_model_radius=
  model_shift=model shift
  search_shift=search shift
  ensemble_search_shift=
  ensemble_model_shift=
  model_rotation=model rotation
  search_rotation=search rotation
  ensemble_search_rotation=
  ensemble_model_rotation=
  search_model_is_fixed=
  fixed_ensemble_search_is_fixed=
  fixed_ensemble_model_is_fixed=
  fixed_model=fixed model
  fixed_search=fixed search
  fixed_ensemble_search=fixed ensemble search
  fixed_ensemble_model=fixed ensemble model
  ensemble_fixed=
  search_fixed=
  ensemble_search_fixed=
  ensemble_model_fixed=
  fixed_ncs_file_name=fixed ncs file name
  fixed_ncs_type=fixed ncs type
  fixed_chain_id=fixed chain id
  fixed_ncs_copies=fixed ncs copies
  fixed_ncs_center=fixed ncs center
  fixed_resolution=fixed resolution
  fixed_density_sigma=1.0 float
  fixed_density_cutoff=0.0 float
  fixed_search_radius=fixed search radius
  fixed_ensemble_search_radius=
  fixed_model_radius=fixed model radius
  fixed_search_shift=fixed search shift
  fixed_ensemble_search_shift=
  fixed_model_shift=fixed model shift
  fixed_search_rotation=fixed search rotation
  fixed_ensemble_search_rotation=
  fixed_model_rotation=fixed model rotation
  fixed_search_copies=fixed search copies
  fixed_ensemble_search_copies=
  fixed_model_copies=fixed model copies
  fixed_search_center=fixed search center
  fixed_ensemble_search_center=
  fixed_model_center=fixed model center
  ncs_file_name=ncs file name
  ncs_type=ncs type
  chain_id=chain id
  resolution=resolution
  density_sigma=1.0 float
  density_cutoff=0.0 float
  search_radius=search radius
  density_sigma=1.0 float
  density_cutoff=0.0 float
  search_radius=search radius
```

```
gff_aln_mrk = False      # Use gff MAG and GAF to annotate, and then run check
                         # Use gff MAG and GAF to annotate
hmm_cut_off = False      # Use the cutoff defined in HMM file to filter out the
                         # Use the cutoff defined in HMM file
cutoff = None            # Cutoff of homology similarity (0-100)
cutoff_cdsnum = None     # Cutoff of number of CDS (integer)
cdsnum = None            # Cut of cdsnum similarity (0-100)
nucleotide = None        # Cut of nucleotide similarity (0-100)
cut_cdsnum_nucleotide_simi = None
                         # Cut of cdsnum nucleotide similarity (0-100)
cut_cdsnum_aa_simi = None
                         # Cut of cdsnum amino acid similarity (0-100)
aln_filtered_simi = None # Aln filtered cut-off similarity (0-100)
cut_filtered_simi = None # Cut filtered cut-off similarity (0-100)
cut_filtered_num = None  # Cut filtered cut-off cdsnum similarity (0-100)
aln_seq_simi = None      # List of aln seq similarity (0-100)
aln_seq_cdsnum = None    # List of aln seq cdsnum similarity (0-100)
aln_seq_aa = None        # List of aln seq amino acid similarity (0-100)
aln_seq_nucleotide = None
                         # List of aln seq nucleotide similarity (0-100)
aln_seq_cut_cdsnum = None
                         # Aln seq cut cdsnum similarity (0-100)
aln_seq_cut_aa = None    # Aln seq cut amino acid similarity (0-100)
aln_seq_cut_nucleotide = None
                         # Aln seq cut nucleotide similarity (0-100)
aln_seq_num = None       # Number of aln seq (integer)
aln_seq_cdsnum = None    # Aln seq cdsnum (integer)
aln_seq_aa = None        # Aln seq amino acid (integer)
aln_seq_nucleotide = None
                         # Aln seq nucleotide (integer)
aln_seq_cut_num = None   # Aln cut seq (integer)
aln_seq_cut_cdsnum = None
                         # Aln cut seq cdsnum (integer)
aln_seq_cut_aa = None    # Aln cut seq amino acid (integer)
aln_seq_cut_nucleotide = None
                         # Aln cut seq nucleotide (integer)
aln_seq_cut_simi = None  # Aln cut seq similarity (0-100)
aln_seq_cut_cdsnum_simi = None
                         # Aln cut seq cdsnum similarity (0-100)
aln_seq_cut_aa_simi = None
                         # Aln cut seq amino acid similarity (0-100)
aln_seq_cut_nucleotide_simi = None
                         # Aln cut seq nucleotide similarity (0-100)
aln_seq_filtered = None  # Aln seq filtered (integer)
aln_seq_filtered_simi = None
                         # Aln seq filtered similarity (0-100)
aln_seq_filtered_num = None
                         # Aln seq filtered cdsnum (integer)
aln_seq_filtered_aa = None
                         # Aln seq filtered amino acid (integer)
aln_seq_filtered_nucleotide = None
                         # Aln seq filtered nucleotide (integer)
aln_seq_cut_filtered = None
                         # Aln cut seq filtered (integer)
aln_seq_cut_filtered_simi = None
                         # Aln cut seq filtered similarity (0-100)
aln_seq_cut_filtered_num = None
                         # Aln cut seq filtered cdsnum (integer)
aln_seq_cut_filtered_aa = None
                         # Aln cut seq filtered amino acid (integer)
aln_seq_cut_filtered_nucleotide = None
                         # Aln cut seq filtered nucleotide (integer)
aln_seq_filtered_cut = None
                         # Aln seq filtered cut (integer)
aln_seq_filtered_cut_simi = None
                         # Aln seq filtered cut similarity (0-100)
aln_seq_filtered_cut_num = None
                         # Aln seq filtered cut cdsnum (integer)
aln_seq_filtered_cut_aa = None
                         # Aln seq filtered cut amino acid (integer)
aln_seq_filtered_cut_nucleotide = None
                         # Aln seq filtered cut nucleotide (integer)
aln_seq_filtered_simi = None
                         # Aln seq filtered similarity (0-100)
aln_seq_filtered_num = None
                         # Aln seq filtered cdsnum (integer)
aln_seq_filtered_aa = None
                         # Aln seq filtered amino acid (integer)
aln_seq_filtered_nucleotide = None
                         # Aln seq filtered nucleotide (integer)
aln_seq_filtered_cut_simi = None
                         # Aln seq filtered cut similarity (0-100)
aln_seq_filtered_cut_num = None
                         # Aln seq filtered cut cdsnum (integer)
aln_seq_filtered_cut_aa = None
                         # Aln seq filtered cut amino acid (integer)
aln_seq_filtered_cut_nucleotide = None
                         # Aln seq filtered cut
```

dock_in_map

Phenix *Python based Hierarchical Environment for Integrated Crystallography*

Docking a model into a cryo-EM map with dock_in_map

Author(s)

- Pavel V. Afonine, Nigel Moriarty

Purpose

The module dock_in_map will automatically dock a model or models into a map.

Uses

How dock_in_map works:

Given a map and model (both are optional) dock_in_map performs the following tasks:

```
  - if the model is not provided (and because without it there nothing to
    do) then a model is created from the map using pdbtools and phenix.
    The model is then used to dock into the map. The created model is
    saved in the output directory with the name <prefix>_from_map.pdb
    (by default prefix is cryo_em)
  - if the model is provided and it is a protein/nucleic/RNA/DNA
    then it is docked into the map using phenix.dock_in_map
  - if the model is not a protein/nucleic/RNA/DNA then it is docked into
    the map using phenix.real_space_refine (if the model is
    ligand/water/ion then the model is placed into the vicinity of the
    map peak)
  - if the model is a protein/nucleic/RNA/DNA then it is
    refined using phenix.real_space_refine
  - Optional silicon-based docking or sampling of ligands and RNA/DNA
    is also available (see the keywords below for details)
  - Optional ligand fitting is also available (see the keywords below
    for details)
  - Full geometry and Ramachandran restraints are used in the
    refinement (see the keywords for details)
  - Optional output of the intermediate results (if requested)
```

Uses

The dock_in_map uses the model to dock into a cryo-EM map and any number of copies of any molecules. You specify the molecules one by one:

```
model=model1.pdb
model=model2.pdb
model=model3.pdb
```

and the number of copies all of once with:

```
nc=1,model1,nc=2,2,2,model2,nc=3,model3
```

to look for 1 copies of model1.pdb, one of model2.pdb and two of model3.pdb.

Alternatively, if the number of copies is unknown dock_in_map will estimate it for you, but you specify the second map with the keyword:

```
search_map=cryo_em_2.ccp4
```

If the second map is provided, dock_in_map, convert it to a pseudo-model that corresponds to the density, and then specify the first pseudo-model and the second pseudo-model (the second pseudo-model is used to estimate the number of copies of the first pseudo-model). Alternatively, if the second density is a pseudo-model, then the number of copies is estimated from the ratio of the number of atoms in two models.

Examples

```
phenix.dock_in_map cryo_em.ccp4 model=model.pdb
```

Standard run of dock_in_map:

```
phenix.dock_in_map cryo_em.ccp4 model=model.pdb
```

Docking model.pdb into cryo_em.ccp4 map. Output files are saved into cryo_em_docking_results_dir/ directory and have prefix cryo_em_docked_model_in_map_*.

```
phenix.dock_in_map cryo_em.ccp4 model=model.pdb nc=2,2,2,model2.pdb
```

Docking model.pdb into cryo_em.ccp4 map. Look for 2 copies of model.pdb and 2 copies of model2.pdb. Output files are saved into cryo_em_docking_results_dir/ directory and have prefix cryo_em_docked_model_in_map_*.

```
phenix.dock_in_map cryo_em.ccp4 model=model.pdb search_map=cryo_em_2.ccp4
```

Docking model.pdb into cryo_em.ccp4 map. Estimate number of copies of model.pdb using cryo_em_2.ccp4 map as a second map. Output files are saved into cryo_em_docking_results_dir/ directory and have prefix cryo_em_docked_model_in_map_*.

Possible Problems

If you have a crystallographic model, density and single-binding will not work properly. You can refine 2F-F model against the map and use the density and the refined model. If you are unsure, you can try Phaser with model, search-ensemble to install the ligand and dock it into the density. Note that if your map is rotated, you will need to rotate the model before using phenix.real_space_refine.

If your model has alternate conformations, only the primary model will be used. Use phenix.pdbtools to remove alternate conformations if you want to use them.

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
ncs_file=None
model=None
  ncs=None
  chain_id=None
  ncs_file=None
  search_model=None
  search_ncs_file=None
  search_chain_id=None
  search_ncs_file=None
  trim_model=None
  target_model=None
  symmetry_file=None
output.title=
  output.dir=cryo_em_docking_results_dir
  output.prefix=cryo_em_docked_model_in_map_*
  output.log_file=cryo_em_docked_model_in_map.log
  output.log=True
  output.cif=True
  output.cif_ligand_restraints=True
  output.cif_ligand_restraints_prefix=ligand_restraints_*
  output.cif_ligand_restraints_merge=True
  output.cif_ligand_restraints_merge_file=ligand_restraints.cif
  output.cif_ligand_restraints_dir=ligand_restraints_dir
  output.intermediate_results=False
  output.write_ncs=False
  output.write_ncs_file=ncs.ncs_spec
  output.write_ncs_chain_id=False
  output.write_ncs_search_model=False
  output.write_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_chain_id=False
  output.write_ncs_search_model_ncs_search_model=False
  output.write_ncs_search_model_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_chain_id=False
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_file=ncs_search_model.ncs_spec
  output.write_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model_ncs_search_model
```

dock_predicted_model

Docking processed AlphaFold and other predicted models in cryo-EM maps

Author(s)

- Dima Lasitsina, Maxim Sousa Fernandes

Purpose

Each predicted model does the domains from a model produced by AlphaFold, ModelTitan and other prediction software in a cryo-EM map. It uses the connectivity of the model as a restraint in the docking process so that the domains are placed in a way that preserves the connectivity of the model as much as possible.

The dock_processed_predicted_model program is normally run directly on an Apollo4 or other cryo-EM processing workstation.

The final step is to process the predicted models to trimming off all the unmatch residues in the predicted models and renumbering the residues from the point of view of each domain.

The next step is to dock each of the domains of the processed model into the map, keeping possible connectivity between the domains of the processed model.

The final step is to accept the processed models into the session and save them to relocate all the parts of the processed model in the cryo-EM map.

Note that you can run all three steps separately with check-only and relaxed.

How dock_predicted_model works:

The model must be dock_predicted_model is a model that is made from four steps starting predicted model. Alternatively, the model can be made from a single step starting from a predicted model, using the command options of predicted models, and the options of predicted models are necessary for the successful dock of the predicted model.

Note that you can work with one chain at a time even if a cryo-EM map that has many chains.

The first step is to dock predicted model to normalize your input predicted or already modified cryo-EM map. It uses the connectivity of the predicted model as a restraint in the docking process.

If you are able to dock your cryo-EM map, keeping only the one representing the region where the model lives (most cryo-EM processing software can do this), the rest of the processing will be much faster. If the map has many chains, this keeping only one chain greatly accelerates the process. If the map has many chains, you should specify all, but you could specify the whole chain, if one map has between the left surrounds and found.

The second step is to dock the predicted model to normalize the cryo-EM map. It uses the connectivity of the predicted model as a restraint in the docking process. The output map is a map that is made from the input map, centered, and fitted into the box of the predicted model. Note that this step may not be perfect, particularly in the case of a very asymmetric molecule. For example, if the predicted model is a long helix, the output map may be shifted in the direction of the helix.

The third step is to dock the domains in the processed model to one and one chain in the map. Each domain is docked and fitted to rigid-body refinement. Then the transformation obtained for that domain is applied to all the other domains in the processed model. Note that this step may not be perfect, particularly in the case of a very asymmetric molecule. For example, if the predicted model is a long helix, the output map may be shifted in the direction of the helix. The fourth step is to accept the processed models into the session and save the output models. Note that this step may not be perfect, particularly in the case of a very asymmetric molecule. For example, if the predicted model is a long helix, the output map may be shifted in the direction of the helix.

Examples

Standard run of dock_predicted_model:

Running dock_predicted_model 6.beta. From the command line you can type:

```
/opt/phenix/phenix-1.21.1-5448/bin/phenix.dock_predicted_model
```

This will write the processed cryo-EM map to dock_2D_final.mrc, dock_processed_pdb.mrc, map_copy.ccp4, 3.ent and dock_processed_pdb.pdb. The output files are in the directory where you ran the command.

Possible Problems :

For unmatched residues, the processed models may not work well because it does not recenter every possible residue in the processed model. Also, the output map may be shifted in the direction of the predicted model. You can improve the processed cryo-EM map and the output models by using the dock_predicted_model command options.

If dock doesn't work, you can try to dock the domains from your AlphaFold model using phenix.dock or map and model. Alternatively, you can try to use the dock_predicted_model command options. For example, you can use the dock_predicted_model command options to dock each domain in the cryo-EM map. Alternatively, you can use the dock_predicted_model command options to dock each domain in the cryo-EM map. Alternatively, you can use the dock_predicted_model command options to dock each domain in the cryo-EM map.

Specific limitations and problems:

Literature

Additional information

List of all available keywords

dock_predicted_model	
[no_check]	Do only a TEMPO DOC, not dock or combine runs
[no_log]	
[no_log_file] = None	Input logfile(s) for Phenix-formatted logfiles (name=filename)
[no_log_file_name] = None	Output logfile name (default: dock_predicted_model.log)
[no_log_file_overwrite] = True	Overwrite existing log file (default: True)
[no_log_file_append] = False	Append to log file (default: False)
[no_log_file_date] = False	Add date/time stamp to log file name (default: False)
[output_model_to_dock_processed_pdb] = dock_processed_pdb.pdb	Output combined model after dock and refine (default: dock_processed_pdb.pdb)
[dock_with_model] = None	Input combined model after dock and refine (default: dock_with_model.pdb)
[dock_2d_final] = None	Output final 2D map after dock and refine (default: dock_2d_final.mrc)
[dock_2d_initial] = None	Output initial 2D map after dock and refine (default: dock_2d_initial.mrc)
[d_cutoff_factor] = 0.5	Factor for cutoff for connectedness (default: 0.5)
[d_cutoff_factor_for_dock] = 0.5	Factor for cutoff for connectedness for dock (default: 0.5)
[dock_fit] = True	Dock and fit domains (default: True)
[dock_fit_only_single_domain] = False	Dock and fit only single domain (default: False)
[dock_fit_only_first_domain] = False	Dock and fit only first domain (default: False)
[dock_fit_only_domain_number] = None	Dock and fit only domain number (default: None)
[dock_fit_only_domain_number_for_dock] = None	Dock and fit only domain number for dock (default: None)
[dock_fit_only_domain_number_for_fit] = None	Dock and fit only domain number for fit (default: None)
[dock_fit_only_domain_number_for_fit_for_dock] = None	Dock and fit only domain number for fit for dock (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit] = None	Dock and fit only domain number for fit for dock for fit (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock] = None	Dock and fit only domain number for fit for dock for fit for dock (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit] = None	Dock and fit only domain number for fit for dock for fit for dock for fit (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock (default: None)
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[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock (default: None)
[dock_fit_only_domain_number_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit_for_dock_for_fit] = None	Dock and fit only domain number for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit for dock for fit

```
[mbstring.language] Default language
                    Specifies the default language, internally in UTF-8, currently used
                    for PHP's multibyte functions. Detection and/or conversion of HTTP input
                    character encoding to this language and internal character encoding to
                    UTF-8 will be done if enabled.
[mbstring.strict]   Enforce strict validation of byte sequences in mbstring functions.
                    Not strict by default.
[mbstring.substitute_character] Specifies substitution character
                    Not changed by default.
[mcrypt.algorithms_dir] Directory where to load mcrypt algorithms
[mcrypt.modes_dir]  Directory where to load mcrypt modes
[mysqlnd.debug]     Comma separated list of mysqlnd trace/debug settings
                    Not checked by default.
[mysqlnd.mempool_default_size] Default size of the mysqlnd memory pool.
                    Not checked by default.
[mysqlnd.net_cmd_buffer_size] Size of a buffer for network commands
[mysqlnd.net_read_buffer_size] Maximum read chunk size in bytes when reading
                    packets over network
[mysqlnd.net_read_timeout] Timeout for network reads
[mysqlnd.sha256_server_public_key] path to RSA public key file for SHA256
                    authentication over non-secure connections
[mysqlnd.trace_alloc] Trace memory allocations, freeds, reallocs and errors
[mysqlnd.trace_mode] Trace protocol events and errors
[mysqlnd.unbuffered_io_buffer_size] Size of a buffer for unbuffered I/O
[mysqlnd.viosocket.dump_dir] Directory for the PHP VIO socket layer to dump
                    network packets to
[mysqlnd.viosocket.dump_header] Dump packet headers when tracing
[mysqlnd.viosocket.dump_size] Maximum number of bytes to dump for each packet
[mysqlnd.viosocket.loop_before_data] Number of iterations to wait for data
                    before aborting an operation
[mysqlnd.viosocket.loop_before_header] Number of iterations to wait for a packet
                    header before aborting an operation
[mysqlnd.viosocket.loop_before_send] Number of iterations to wait before aborting
                    a send operation
[mysqlnd.viosocket.loop_before_time] Time in seconds to wait before aborting an
                    operation
[mysqlnd.zval_cache_enabled] Enable or disable the zval cache
[mysqlnd.zval_cache_size] Size of the zval cache
[mysqlnd.zval_cache_type] Type of the zval cache (0 = per-request, 1 = persistent)
[mysqlnd.zval_cache_validation] Enable or disable validation of the zval cache
[nsd.chroot]        Chroot directory
[nsd.cookie]        Cookie for the server
[nsd.dbfile]        Database file
[nsd.debug]         Debugging level
[nsd.ipv4address]   IPv4 address to bind to
[nsd.ipv6address]   IPv6 address to bind to
[nsd.nosd]          Path to nsd executable
[nsd.pidfile]       Pid file
[nsd.port]          Port number
[nsd.statistics]    Statistics interval
[nsd.zonefiles]     Zone files
[nsd.zonelist]      Zone list
[nsd.zonesdir]      Zones directory
[nsd.zonestat]      Zone statistics
[nsd.zonesubnets]   Allowed zone subnets
[nsd.zonetimeout]   Zone timeout
[nsd.zonewrite]     Zone write interval
[nsd.zonexfrd]      Path to zonexfrd executable
[nsd.zonexfrdfile]  Zone transfer file
[nsd.zonexfrdport]  Zone transfer port
[nsd.zonexfrdsubnets] Zone transfer subnets
[nsd.zonexfrdtimeout] Zone transfer timeout
[nsd.zonexfrdtmp]   Temporary directory for zone transfers
[nsd.zonexfrdtmpfile] Temporary file for zone transfer
[nsd.zonexfrdtmpfilesize] Maximum size of temporary file for zone transfer
[nsd.zonexfrdtmpfilesizeexp] Exponent for maximum size of temporary file for
                    zone transfer
[nsd.zonexfrdtmpfilesizemant] Mantissa for maximum size of temporary file for
                    zone transfer
[nsd.zonexfrdtmpfilesizeunit] Unit for maximum size of temporary file for
                    zone transfer
[nsd.zonexfrdtmpfilesizeunitnum] Numeric unit for maximum size of temporary file
                    for zone transfer
[nsd.zonexfrdtmpfilesizeunitstr] String unit for maximum size of temporary file
                    for zone transfer
[nsd.zonexfrdtmpfilesizeunitstrlen] Length of string unit for maximum size of
                    temporary file for zone transfer
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                    maximum size of temporary file for zone transfer
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                    unit for maximum size of temporary file for zone transfer
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                    for zone transfer
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```

Solid water into cryo-EM map using phenix.dusse

phenix.dusse [--help] [--show-defaults] [--version] model.pdb map.ccp4

Facts about the procedure

1) The water is built into density map step wise(one water is linked to the protein no h bond, directly or through water molecule).

2) density height of the water molecule is assumed to be as complete and possible as possible (for example, 6 Sigma was refined individually).

3) Water is placed in the center of a grid cube enclosing our three two protein surfaces. This allows to build about the solvent layers around protein. The unmodeled density in the region is marked as potential water.

4) Minimal (2a0, one) and maximal (2a0, two) distance between any water and protein or other water are 2 and 3.5 A respectively (default).

5) Not all protein atoms are used to assess contacts with prospective water molecules but only those that are within 5 A from the current water. Water molecule is placed in the center of a cube with 5 A edge and placed in the map. The confidence is quantified by Crowet by, chain threshold (averaging phenix. , the minimum of the average density in the chain and the density at the water position) and the density is 0.5. The Chimera is calculated in sphere of 4A below atom, centred around the atom in question.

6) Only strong enough density peaks are considered as potential water candidates. "Strong enough" is defined by the user as a fraction of the chain density. Default is 0.5 (50%). Only those water molecules with density above the specified fraction are considered as potential water candidates.

7) The new molecule gets a chain name from a pool of available chain names.

Use as Chimera (or, chain) PDB with the cutoff value of 0.5 (i.e., chain threshold). The Chimera is calculated in sphere of 4A below atom, centred around the atom in question. Only those water molecules with density above unassigned density are kept. Unassigned density is performed for newly added water molecules.

Another selection criterion is peak sphericity (psphr). The peak sphericity is evaluated as minimal correlation between density in a given point and a set of spherical functions centred in the point. Only those peaks with sphericity height of 0.75 or higher are selected when the correlation between only "peak of spherical" and peak of density is used. Sphericity filter factors (field no. 7 PDB) is applied if no a the Mult 0.75.

Comments

1) Sphericity (psphr) problem of water solvent distance and chemical bonding of interacting atoms criteria are rather strong and high criteria and do not allow much room for variation. The set default values are taken from Phenix manuals.

2) Map-based criteria, such as sphericity (psphr), are very tolerant and rule out of the bulk water. For example, the default value of 0.75 for sphericity (psphr) rules out 50% of the bulk water. For well resolved water sites(e.g. half way between more and perfect). Choosing a larger value will mean choosing more confident water sites.

3) Map sphericity reflects the observation that water density supports to be approximately spherical most of the time. Sphericity (psphr) is a good criterion to distinguish between water and other molecules. Sphericity is a measure of local improvement of the map. For example, at high resolution water with high structural mobility may not be spherical in density. Sphericity (psphr) is a good criterion to be used for water identification and peak or even if maximal or minimal point is sphericity can be largely polarized.

4) Peak height threshold for selecting peak candidates is another rather ad hoc criterion. It uses peak heights of the density map to select water candidates. Peak height threshold is a fraction of the chain density. Default is 0.5 (50%). Only those water molecules with density above the specified fraction are considered as potential water candidates. Peak height threshold is a fraction of the chain density.

5) Building large water vertices such as water or ions is a much more difficult task to be correspond to building a water molecule. Water molecule is a small molecule with a well defined structure. Water molecule is a small molecule with well defined structure and well defined density. Chemical bonding and distance criteria are a much more reliable criteria for identification of water molecules. Chemical bonding and distance criteria are a much more reliable criteria. Therefore, better building procedure is unlikely to be more fully automated.

Availability

Command line, GUI

Required inputs

phenix model (PDB or mmCIF format) and map (MRC format).

resolution is required if.a.map_filter is set to True.

Optional inputs

resolution

map = phenix.ccp4_map(file_name=map_name, resolution=2.1)

sphericity_filter = True: use peak sphericity criteria. Disabled by default.

sphericity_cutoff = 0.75: map peak sphericity characteristic. Decreases to add more water.

sphericity_radius = 1.5: radius of sphere for sphericity.

peak_cutoff = 0.5: minimal peak value to add water atom. Decreases to add more water.

peak_radius = 0.25: maximal peak value to add water atom. Decreases to add more water.

cutoff = 0.5: map to averaging ratio

map_threshold_cutoff = 0.5: map threshold for water selection = (mean map value at atom centers) * map_threshold_cutoff. Decreases to add more water.

a_map_filter = True: input water with CC_peak >.a_map_filter_threshold.

a_map_filter_threshold = 0.5 CC_peak threshold for capturing water.

resolution: map resolution. Required if a_map_filter=True

Limitations

Only orthorhombic and fully expanded symmetry.

Assumptions

Macromolecular part of the phenix model is as complete as possible (no missing chains or other unmodelled macromolecules). Ions are not modelled (only water molecules are modelled).

Map resolution is sufficiently high to expect water oxygens be visible in the map.

Example

phenix.dusse model.pdb map.mrc resolution=2.1

resolution is required if.a.map_filter is set to True.

More information

https://www.ccp4.ac.uk/dist/macosarm64_latest/manuals/files/examinations/water.pdf

Please refer to the documentation at the top of drawing file (dusse.dwg). The procedure is most current version of dusse.dwg. Use at your own risk.

Author

Vuk Mirdita (VMirdita@hhu.pro)

phenix.dynamics: simple model perturbation

Python-based Hierarchical ATomistic Model Building and Refinement for Enhanced Cryo-EM Modeling

This program performs rigid bodies dynamics in a cartesian coordinate system. The program accepts any PDB file and any CIF file with bond, angle, dihedral, chirality, planarity, and non-bonded nonbonded interactions. Due to the lack of attractive force such as electrostatic, and solvent, only small steps of minimization can be made. The program is intended to perform small-scale structure perturbation.

The program uses the cartesian coordinate system and the Verlet integration scheme. The forces for the potential energy are calculated using the gradients of the bond, angle, dihedral, chirality, planarity, and non-bonded nonbonded interactions. The forces are in kcal/mol and are Gaussians distributed. [Cf.] Thus, the kinetic energy of the system is in units of kcal/mol. The kinetic energy is calculated using the equipartition theorem. Since the system is in an isolated thermodynamic ensemble, the model will drift to a certain region of high temperatures.

Alternatives and complementary programs

- phenix.geometry_minimization can be used to perform small-scale structure minimization. Unlike phenix.dynamics,

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    # Leave empty to use OpenRouter free tier (rate limited)
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    # Together.ai offers Qwen3-Coder-Flash with function calling
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    # Get your key at https://together.ai/
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    # Parasail offers Qwen3-Coder-Flash with function calling
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    # Get your key at https://parasail.io/
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    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
    # Enable Together.ai provider
    # Together.ai offers Qwen3-32B with function calling
    "together_enable": false
    # Together.ai API key
    # Get your key at https://together.ai/
    "together_api_key": ""
    # Together.ai model to use
    # Recommended: Qwen/Qwen3-32B-FP8 for function calling
    "together_model": "Qwen/Qwen3-32B-FP8"
    # Enable Groq provider
    # Groq offers fast inference for Qwen3-32B
    "groq_enable": false
    # Groq API key
    # Get your key at https://console.groq.com/
    "groq_api_key": ""
    # Groq model to use
    # Recommended: qwen/qwen3-32b for function calling
    "groq_model": "qwen/qwen3-32b"
    # Enable Fireworks provider
    # Fireworks offers Qwen3-32B with function calling
    "fireworks_enable": false
    # Fireworks API key
    # Get your key at https://fireworks.ai/
    "fireworks_api_key": ""
    # Fireworks model to use
    # Recommended: accounts/fireworks/models/qwen3-32b for function calling
    "fireworks_model": "accounts/fireworks/models/qwen3-32b"
    # Enable Chutes provider
    # Chutes offers Qwen3-32B with function calling
    "chutes_enable": false
    # Chutes API key
    # Get your key at https://chutes.ai/
    "chutes_api_key": ""
    # Chutes model to use
    # Recommended: Qwen/Qwen3-32B for function calling
    "chutes_model": "Qwen/Qwen3-32B"
    # Enable Nebius provider
    # Nebius offers Qwen3-32B with function calling
    "nebius_enable": false
    # Nebius API key
    # Get your key at https://nebius.com/
    "nebius_api_key": ""
    # Nebius model to use
    # Recommended: Qwen/Qwen3-32B-fast for function calling
    "nebius_model": "Qwen/Qwen3-32B-fast"
    # Enable Novita provider
    # Novita offers Qwen3-32B with function calling
    "novita_enable": false
    # Novita API key
    # Get your key at https://novita.ai/
    "novita_api_key": ""
    # Novita model to use
    # Recommended: qwen/qwen3-32b-fp8 for function calling
    "novita_model": "qwen/qwen3-32b-fp8"
    # Enable Parasail provider
    # Parasail offers Qwen3-32B with function calling
    "parasail_enable": false
    # Parasail API key
    # Get your key at https://parasail.io/
    "parasail_api_key": ""
    # Parasail model to use
    # Recommended: parasail-qwen3-32b for function calling
    "parasail_model": "parasail-qwen3-32b"
    # Enable SambaNova provider
    # SambaNova offers Qwen3-32B with function calling
    "sambanova_enable": false
    # SambaNova API key
    # Get your key at https://sambanova.ai/
    "sambanova_api_key": ""
    # SambaNova model to use
    # Recommended: Qwen3-32B for function calling
    "sambanova_model": "Qwen3-32B"
  "cerebras_qwen3":
    "enable": true
    "max_tokens": 4096
    "temperature": 0.7
    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
    # Enable Together.ai provider
    # Together.ai offers Qwen3-32B with function calling
    "together_enable": false
    # Together.ai API key
    # Get your key at https://together.ai/
    "together_api_key": ""
    # Together.ai model to use
    # Recommended: Qwen/Qwen3-32B-FP8 for function calling
    "together_model": "Qwen/Qwen3-32B-FP8"
    # Enable Groq provider
    # Groq offers fast inference for Qwen3-32B
    "groq_enable": false
    # Groq API key
    # Get your key at https://console.groq.com/
    "groq_api_key": ""
    # Groq model to use
    # Recommended: qwen/qwen3-32b for function calling
    "groq_model": "qwen/qwen3-32b"
    # Enable Fireworks provider
    # Fireworks offers Qwen3-32B with function calling
    "fireworks_enable": false
    # Fireworks API key
    # Get your key at https://fireworks.ai/
    "fireworks_api_key": ""
    # Fireworks model to use
    # Recommended: accounts/fireworks/models/qwen3-32b for function calling
    "fireworks_model": "accounts/fireworks/models/qwen3-32b"
    # Enable Chutes provider
    # Chutes offers Qwen3-32B with function calling
    "chutes_enable": false
    # Chutes API key
    # Get your key at https://chutes.ai/
    "chutes_api_key": ""
    # Chutes model to use
    # Recommended: Qwen/Qwen3-32B for function calling
    "chutes_model": "Qwen/Qwen3-32B"
    # Enable Nebius provider
    # Nebius offers Qwen3-32B with function calling
    "nebius_enable": false
    # Nebius API key
    # Get your key at https://nebius.com/
    "nebius_api_key": ""
    # Nebius model to use
    # Recommended: Qwen/Qwen3-32B-fast for function calling
    "nebius_model": "Qwen/Qwen3-32B-fast"
    # Enable Novita provider
    # Novita offers Qwen3-32B with function calling
    "novita_enable": false
    # Novita API key
    # Get your key at https://novita.ai/
    "novita_api_key": ""
    # Novita model to use
    # Recommended: qwen/qwen3-32b-fp8 for function calling
    "novita_model": "qwen/qwen3-32b-fp8"
    # Enable Parasail provider
    # Parasail offers Qwen3-32B with function calling
    "parasail_enable": false
    # Parasail API key
    # Get your key at https://parasail.io/
    "parasail_api_key": ""
    # Parasail model to use
    # Recommended: parasail-qwen3-32b for function calling
    "parasail_model": "parasail-qwen3-32b"
    # Enable SambaNova provider
    # SambaNova offers Qwen3-32B with function calling
    "sambanova_enable": false
    # SambaNova API key
    # Get your key at https://sambanova.ai/
    "sambanova_api_key": ""
    # SambaNova model to use
    # Recommended: Qwen3-32B for function calling
    "sambanova_model": "Qwen3-32B"
  "cerebras_glm":
    "enable": true
    "max_tokens": 4096
    "temperature": 0.7
    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
    # Enable Together.ai provider
    # Together.ai offers Qwen3-32B with function calling
    "together_enable": false
    # Together.ai API key
    # Get your key at https://together.ai/
    "together_api_key": ""
    # Together.ai model to use
    # Recommended: Qwen/Qwen3-32B-FP8 for function calling
    "together_model": "Qwen/Qwen3-32B-FP8"
    # Enable Groq provider
    # Groq offers fast inference for Qwen3-32B
    "groq_enable": false
    # Groq API key
    # Get your key at https://console.groq.com/
    "groq_api_key": ""
    # Groq model to use
    # Recommended: qwen/qwen3-32b for function calling
    "groq_model": "qwen/qwen3-32b"
    # Enable Fireworks provider
    # Fireworks offers Qwen3-32B with function calling
    "fireworks_enable": false
    # Fireworks API key
    # Get your key at https://fireworks.ai/
    "fireworks_api_key": ""
    # Fireworks model to use
    # Recommended: accounts/fireworks/models/qwen3-32b for function calling
    "fireworks_model": "accounts/fireworks/models/qwen3-32b"
    # Enable Chutes provider
    # Chutes offers Qwen3-32B with function calling
    "chutes_enable": false
    # Chutes API key
    # Get your key at https://chutes.ai/
    "chutes_api_key": ""
    # Chutes model to use
    # Recommended: Qwen/Qwen3-32B for function calling
    "chutes_model": "Qwen/Qwen3-32B"
    # Enable Nebius provider
    # Nebius offers Qwen3-32B with function calling
    "nebius_enable": false
    # Nebius API key
    # Get your key at https://nebius.com/
    "nebius_api_key": ""
    # Nebius model to use
    # Recommended: Qwen/Qwen3-32B-fast for function calling
    "nebius_model": "Qwen/Qwen3-32B-fast"
    # Enable Novita provider
    # Novita offers Qwen3-32B with function calling
    "novita_enable": false
    # Novita API key
    # Get your key at https://novita.ai/
    "novita_api_key": ""
    # Novita model to use
    # Recommended: qwen/qwen3-32b-fp8 for function calling
    "novita_model": "qwen/qwen3-32b-fp8"
    # Enable Parasail provider
    # Parasail offers Qwen3-32B with function calling
    "parasail_enable": false
    # Parasail API key
    # Get your key at https://parasail.io/
    "parasail_api_key": ""
    # Parasail model to use
    # Recommended: parasail-qwen3-32b for function calling
    "parasail_model": "parasail-qwen3-32b"
    # Enable SambaNova provider
    # SambaNova offers Qwen3-32B with function calling
    "sambanova_enable": false
    # SambaNova API key
    # Get your key at https://sambanova.ai/
    "sambanova_api_key": ""
    # SambaNova model to use
    # Recommended: Qwen3-32B for function calling
    "sambanova_model": "Qwen3-32B"
  "cerebras_gpt_oss":
    "enable": true
    "max_tokens": 4096
    "temperature": 0.7
    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
    # Enable Together.ai provider
    # Together.ai offers Qwen3-32B with function calling
    "together_enable": false
    # Together.ai API key
    # Get your key at https://together.ai/
    "together_api_key": ""
    # Together.ai model to use
    # Recommended: Qwen/Qwen3-32B-FP8 for function calling
    "together_model": "Qwen/Qwen3-32B-FP8"
    # Enable Groq provider
    # Groq offers fast inference for Qwen3-32B
    "groq_enable": false
    # Groq API key
    # Get your key at https://console.groq.com/
    "groq_api_key": ""
    # Groq model to use
    # Recommended: qwen/qwen3-32b for function calling
    "groq_model": "qwen/qwen3-32b"
    # Enable Fireworks provider
    # Fireworks offers Qwen3-32B with function calling
    "fireworks_enable": false
    # Fireworks API key
    # Get your key at https://fireworks.ai/
    "fireworks_api_key": ""
    # Fireworks model to use
    # Recommended: accounts/fireworks/models/qwen3-32b for function calling
    "fireworks_model": "accounts/fireworks/models/qwen3-32b"
    # Enable Chutes provider
    # Chutes offers Qwen3-32B with function calling
    "chutes_enable": false
    # Chutes API key
    # Get your key at https://chutes.ai/
    "chutes_api_key": ""
    # Chutes model to use
    # Recommended: Qwen/Qwen3-32B for function calling
    "chutes_model": "Qwen/Qwen3-32B"
    # Enable Nebius provider
    # Nebius offers Qwen3-32B with function calling
    "nebius_enable": false
    # Nebius API key
    # Get your key at https://nebius.com/
    "nebius_api_key": ""
    # Nebius model to use
    # Recommended: Qwen/Qwen3-32B-fast for function calling
    "nebius_model": "Qwen/Qwen3-32B-fast"
    # Enable Novita provider
    # Novita offers Qwen3-32B with function calling
    "novita_enable": false
    # Novita API key
    # Get your key at https://novita.ai/
    "novita_api_key": ""
    # Novita model to use
    # Recommended: qwen/qwen3-32b-fp8 for function calling
    "novita_model": "qwen/qwen3-32b-fp8"
    # Enable Parasail provider
    # Parasail offers Qwen3-32B with function calling
    "parasail_enable": false
    # Parasail API key
    # Get your key at https://parasail.io/
    "parasail_api_key": ""
    # Parasail model to use
    # Recommended: parasail-qwen3-32b for function calling
    "parasail_model": "parasail-qwen3-32b"
    # Enable SambaNova provider
    # SambaNova offers Qwen3-32B with function calling
    "sambanova_enable": false
    # SambaNova API key
    # Get your key at https://sambanova.ai/
    "sambanova_api_key": ""
    # SambaNova model to use
    # Recommended: Qwen3-32B for function calling
    "sambanova_model": "Qwen3-32B"
  "cerebras_qwen3_coder":
    "enable": true
    "max_tokens": 4096
    "temperature": 0.7
    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
    # Enable Together.ai provider
    # Together.ai offers Qwen3-32B with function calling
    "together_enable": false
    # Together.ai API key
    # Get your key at https://together.ai/
    "together_api_key": ""
    # Together.ai model to use
    # Recommended: Qwen/Qwen3-32B-FP8 for function calling
    "together_model": "Qwen/Qwen3-32B-FP8"
    # Enable Groq provider
    # Groq offers fast inference for Qwen3-32B
    "groq_enable": false
    # Groq API key
    # Get your key at https://console.groq.com/
    "groq_api_key": ""
    # Groq model to use
    # Recommended: qwen/qwen3-32b for function calling
    "groq_model": "qwen/qwen3-32b"
    # Enable Fireworks provider
    # Fireworks offers Qwen3-32B with function calling
    "fireworks_enable": false
    # Fireworks API key
    # Get your key at https://fireworks.ai/
    "fireworks_api_key": ""
    # Fireworks model to use
    # Recommended: accounts/fireworks/models/qwen3-32b for function calling
    "fireworks_model": "accounts/fireworks/models/qwen3-32b"
    # Enable Chutes provider
    # Chutes offers Qwen3-32B with function calling
    "chutes_enable": false
    # Chutes API key
    # Get your key at https://chutes.ai/
    "chutes_api_key": ""
    # Chutes model to use
    # Recommended: Qwen/Qwen3-32B for function calling
    "chutes_model": "Qwen/Qwen3-32B"
    # Enable Nebius provider
    # Nebius offers Qwen3-32B with function calling
    "nebius_enable": false
    # Nebius API key
    # Get your key at https://nebius.com/
    "nebius_api_key": ""
    # Nebius model to use
    # Recommended: Qwen/Qwen3-32B-fast for function calling
    "nebius_model": "Qwen/Qwen3-32B-fast"
    # Enable Novita provider
    # Novita offers Qwen3-32B with function calling
    "novita_enable": false
    # Novita API key
    # Get your key at https://novita.ai/
    "novita_api_key": ""
    # Novita model to use
    # Recommended: qwen/qwen3-32b-fp8 for function calling
    "novita_model": "qwen/qwen3-32b-fp8"
    # Enable Parasail provider
    # Parasail offers Qwen3-32B with function calling
    "parasail_enable": false
    # Parasail API key
    # Get your key at https://parasail.io/
    "parasail_api_key": ""
    # Parasail model to use
    # Recommended: parasail-qwen3-32b for function calling
    "parasail_model": "parasail-qwen3-32b"
    # Enable SambaNova provider
    # SambaNova offers Qwen3-32B with function calling
    "sambanova_enable": false
    # SambaNova API key
    # Get your key at https://sambanova.ai/
    "sambanova_api_key": ""
    # SambaNova model to use
    # Recommended: Qwen3-32B for function calling
    "sambanova_model": "Qwen3-32B"
  "cerebras_qwen3_coder_480b":
    "enable": true
    "max_tokens": 4096
    "temperature": 0.7
    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
    # Enable Together.ai provider
    # Together.ai offers Qwen3-32B with function calling
    "together_enable": false
    # Together.ai API key
    # Get your key at https://together.ai/
    "together_api_key": ""
    # Together.ai model to use
    # Recommended: Qwen/Qwen3-32B-FP8 for function calling
    "together_model": "Qwen/Qwen3-32B-FP8"
    # Enable Groq provider
    # Groq offers fast inference for Qwen3-32B
    "groq_enable": false
    # Groq API key
    # Get your key at https://console.groq.com/
    "groq_api_key": ""
    # Groq model to use
    # Recommended: qwen/qwen3-32b for function calling
    "groq_model": "qwen/qwen3-32b"
    # Enable Fireworks provider
    # Fireworks offers Qwen3-32B with function calling
    "fireworks_enable": false
    # Fireworks API key
    # Get your key at https://fireworks.ai/
    "fireworks_api_key": ""
    # Fireworks model to use
    # Recommended: accounts/fireworks/models/qwen3-32b for function calling
    "fireworks_model": "accounts/fireworks/models/qwen3-32b"
    # Enable Chutes provider
    # Chutes offers Qwen3-32B with function calling
    "chutes_enable": false
    # Chutes API key
    # Get your key at https://chutes.ai/
    "chutes_api_key": ""
    # Chutes model to use
    # Recommended: Qwen/Qwen3-32B for function calling
    "chutes_model": "Qwen/Qwen3-32B"
    # Enable Nebius provider
    # Nebius offers Qwen3-32B with function calling
    "nebius_enable": false
    # Nebius API key
    # Get your key at https://nebius.com/
    "nebius_api_key": ""
    # Nebius model to use
    # Recommended: Qwen/Qwen3-32B-fast for function calling
    "nebius_model": "Qwen/Qwen3-32B-fast"
    # Enable Novita provider
    # Novita offers Qwen3-32B with function calling
    "novita_enable": false
    # Novita API key
    # Get your key at https://novita.ai/
    "novita_api_key": ""
    # Novita model to use
    # Recommended: qwen/qwen3-32b-fp8 for function calling
    "novita_model": "qwen/qwen3-32b-fp8"
    # Enable Parasail provider
    # Parasail offers Qwen3-32B with function calling
    "parasail_enable": false
    # Parasail API key
    # Get your key at https://parasail.io/
    "parasail_api_key": ""
    # Parasail model to use
    # Recommended: parasail-qwen3-32b for function calling
    "parasail_model": "parasail-qwen3-32b"
    # Enable SambaNova provider
    # SambaNova offers Qwen3-32B with function calling
    "sambanova_enable": false
    # SambaNova API key
    # Get your key at https://sambanova.ai/
    "sambanova_api_key": ""
    # SambaNova model to use
    # Recommended: Qwen3-32B for function calling
    "sambanova_model": "Qwen3-32B"
  "cerebras_glm_4_6":
    "enable": true
    "max_tokens": 4096
    "temperature": 0.7
    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
    # Enable Together.ai provider
    # Together.ai offers Qwen3-32B with function calling
    "together_enable": false
    # Together.ai API key
    # Get your key at https://together.ai/
    "together_api_key": ""
    # Together.ai model to use
    # Recommended: Qwen/Qwen3-32B-FP8 for function calling
    "together_model": "Qwen/Qwen3-32B-FP8"
    # Enable Groq provider
    # Groq offers fast inference for Qwen3-32B
    "groq_enable": false
    # Groq API key
    # Get your key at https://console.groq.com/
    "groq_api_key": ""
    # Groq model to use
    # Recommended: qwen/qwen3-32b for function calling
    "groq_model": "qwen/qwen3-32b"
    # Enable Fireworks provider
    # Fireworks offers Qwen3-32B with function calling
    "fireworks_enable": false
    # Fireworks API key
    # Get your key at https://fireworks.ai/
    "fireworks_api_key": ""
    # Fireworks model to use
    # Recommended: accounts/fireworks/models/qwen3-32b for function calling
    "fireworks_model": "accounts/fireworks/models/qwen3-32b"
    # Enable Chutes provider
    # Chutes offers Qwen3-32B with function calling
    "chutes_enable": false
    # Chutes API key
    # Get your key at https://chutes.ai/
    "chutes_api_key": ""
    # Chutes model to use
    # Recommended: Qwen/Qwen3-32B for function calling
    "chutes_model": "Qwen/Qwen3-32B"
    # Enable Nebius provider
    # Nebius offers Qwen3-32B with function calling
    "nebius_enable": false
    # Nebius API key
    # Get your key at https://nebius.com/
    "nebius_api_key": ""
    # Nebius model to use
    # Recommended: Qwen/Qwen3-32B-fast for function calling
    "nebius_model": "Qwen/Qwen3-32B-fast"
    # Enable Novita provider
    # Novita offers Qwen3-32B with function calling
    "novita_enable": false
    # Novita API key
    # Get your key at https://novita.ai/
    "novita_api_key": ""
    # Novita model to use
    # Recommended: qwen/qwen3-32b-fp8 for function calling
    "novita_model": "qwen/qwen3-32b-fp8"
    # Enable Parasail provider
    # Parasail offers Qwen3-32B with function calling
    "parasail_enable": false
    # Parasail API key
    # Get your key at https://parasail.io/
    "parasail_api_key": ""
    # Parasail model to use
    # Recommended: parasail-qwen3-32b for function calling
    "parasail_model": "parasail-qwen3-32b"
    # Enable SambaNova provider
    # SambaNova offers Qwen3-32B with function calling
    "sambanova_enable": false
    # SambaNova API key
    # Get your key at https://sambanova.ai/
    "sambanova_api_key": ""
    # SambaNova model to use
    # Recommended: Qwen3-32B for function calling
    "sambanova_model": "Qwen3-32B"
  "cerebras_qwen3_235b":
    "enable": true
    "max_tokens": 4096
    "temperature": 0.7
    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
    # Enable Together.ai provider
    # Together.ai offers Qwen3-32B with function calling
    "together_enable": false
    # Together.ai API key
    # Get your key at https://together.ai/
    "together_api_key": ""
    # Together.ai model to use
    # Recommended: Qwen/Qwen3-32B-FP8 for function calling
    "together_model": "Qwen/Qwen3-32B-FP8"
    # Enable Groq provider
    # Groq offers fast inference for Qwen3-32B
    "groq_enable": false
    # Groq API key
    # Get your key at https://console.groq.com/
    "groq_api_key": ""
    # Groq model to use
    # Recommended: qwen/qwen3-32b for function calling
    "groq_model": "qwen/qwen3-32b"
    # Enable Fireworks provider
    # Fireworks offers Qwen3-32B with function calling
    "fireworks_enable": false
    # Fireworks API key
    # Get your key at https://fireworks.ai/
    "fireworks_api_key": ""
    # Fireworks model to use
    # Recommended: accounts/fireworks/models/qwen3-32b for function calling
    "fireworks_model": "accounts/fireworks/models/qwen3-32b"
    # Enable Chutes provider
    # Chutes offers Qwen3-32B with function calling
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    "parasail_enable": false
    # Parasail API key
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    # Parasail model to use
    # Recommended: parasail-qwen3-32b for function calling
    "parasail_model": "parasail-qwen3-32b"
    # Enable SambaNova provider
    # SambaNova offers Qwen3-32B with function calling
    "sambanova_enable": false
    # SambaNova API key
    # Get your key at https://sambanova.ai/
    "sambanova_api_key": ""
    # SambaNova model to use
    # Recommended: Qwen3-32B for function calling
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  "cerebras_qwen3_235b_thinking":
    "enable": true
    "max_tokens": 4096
    "temperature": 0.7
    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
    # Enable Together.ai provider
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    "parasail_model": "parasail-qwen3-32b"
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    # SambaNova offers Qwen3-32B with function calling
    "sambanova_enable": false
    # SambaNova API key
    # Get your key at https://sambanova.ai/
    "sambanova_api_key": ""
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    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
    # Enable Together.ai provider
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    # Get your key at https://sambanova.ai/
    "sambanova_api_key": ""
    # SambaNova model to use
    # Recommended: Qwen3-32B for function calling
    "sambanova_model": "Qwen3-32B"
  "cerebras_qwen3_235b_instruct_fast":
    "enable": true
    "max_tokens": 4096
    "temperature": 0.7
    "reasoning_effort": "medium"
    # Cerebras API key
    # Get your key at https://cerebras.ai/
    "cerebras_api_key": ""
    # Cerebras model to use
    # Available models: qwen-3-32b, llama3.1-8b, llama-3.3-70b, gpt-oss-120b
    "cerebras_model": "qwen-3-32b"
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    # Together.ai API key
    # Get your key at https://together.ai/
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    # Groq API key
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    # Fireworks API key
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    "fireworks_model": "accounts/fireworks/models/qwen3-32b"
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    # Chutes offers Qwen3-32B with function calling
    "chutes_enable": false
    # Chutes API key
    # Get your key at https://chutes.ai/
    "chutes_api_key": ""
    # Chutes model to use
    # Recommended: Qwen/Qwen3-32B for function calling
    "chutes_model": "Qw
```

Phenix

Macromolecular Structure Determination for Integrated Biology

electronic Ligand Builder and Optimization Workbench (eLBOW)

Contents

- Author
- Purpose
- Video Tutorial
- Examples
  - PDB input
  - Other input
  - Geometry optimization
- Advanced options
  - Chiral
  - CIs/Trans
  - Rotamer
  - Geometry optimization
- Output
  - Output files
  - Log file
  - Cif file
  - Pdb file
- Keywords
  - Input
  - Output
  - Geometry optimization
  - Chiral options
  - Rotamer options
  - Cis/trans options

Author

Nigel W. Moriarty

Purpose

Automatic high quality generation of chemically valid coordinates for millions(!) of small ligands and chemical accessories like protein modifications and modified bases. A powerful command line program that can process and manipulate chemical data in a variety of formats. Can be used to generate ligand restraints for refinement, to add hydrogens and other missing atoms to ligands, to convert chemical formats, to generate conformers, to optimize geometry, to add or remove chiral centers, to add or remove cis/trans isomers, to add or remove rotamers, to generate ligand conformer libraries, to generate ligand conformer libraries, to add or remove rotamers, to generate ligand conformer libraries, to add or remove rotamers, to generate ligand conformer libraries, to add or remove rotamers

The "Accessories" option will write a molecule (CIF) and geometry (PDB) file for each permutation of the ligand and metal cofactors in the current directory, using the current molecule name as a prefix. The ligand and metal cofactors are taken from the molecule contained in the system. Cofactor files are written into the subdirectory of the current directory specified by the "Cofactor directory" option, which defaults to the current directory if not specified.

The definition of the 6 and 5 coordinate distributions. Consider a ring in the chair configuration. At one atom in the ring, there are two axial and two equatorial positions. Number it as 1. Go equatorial, 2. Move downhill, axial, 3. Go the ring pucker and otherwise.

To fix a ring into a specific pucker, use Ring. The atoms after configuration of the pucker group use the Ring numbering.

Additional programs

- phenix.pdb_chain
- phenix.ligand
- phenix.ccp4_cif_validation - Generate edits for metal coordination
- phenix.ccp4_cif_modification - Apply edits from PDB-CSD services
- phenix.phenix_geometryo
- phenix.phenix_geometry
- phenix.phenix_cif
- phenix.convert_cif - Molecules
- phenix.convert_pdb
- phenix.pdb_tools
- phenix.pdb_chain_extract
- phenix.phenix_fetch_cif - Fetch CIF files from PDB-CSD services
- phenix.phenix_fetch_pdb

Literature

Grabowski M, Macindoe G, Cronin SR, Karlus DR, **phenix.ligand Builder and Optimization Workbench (LIGAND) for the Phenix suite: from macromolecular cryo-EM models to publication-quality ligands**, Nucleic Acids Res. 2025 Jul 7;53(W1):W64-W75. doi: 10.1093/nar/gkaf409. PMID: 40463247; PMCID: PMC12280811.

Additional information

Novice options

Option	Default & choices	Description of inputs and uses
output_dir	None	Base directory where output files are put
hetp	None	Input file with HETATM and ATOM
hetp_file	None	Input file with HETATM and ATOM
ligand_name	None	Ligand name to be used in output files
cif	*	cif file for chemical CIF
cif_dir	None	Directory with chemical CIF files
mol	None	Input file with molecule for chemical data
mol_dir	None	Directory with molecule for chemical data
chemical component	None	Input name from chemical components
pdb	None	Input chain from standard in
chain	*	Chain to be used in the HETATM
resno	*	The residue number to be used in the HETATM
sequence	*	Sequence to be used in the HETATM
model only	None	Add the ligand but skip all else
cif only	None	Add the ligand but skip all else
metadata	*	Metadata to be passed to the scoring and filtering
changes	*	Changes to be made to the ligand
ignoreal	None	Ignore alternate locations
options	None	Options for ligand Builder and Optimization Workbench
ptorsion	None	Torsion for the ligand to be focused on (starting)
ftor geometry	None	Force torsion to be used in geometry
ftor2 geometry	None	Force torsion 2 to be used in geometry
ensrep validation	None	Run ensemble refinement validation and find ensemble
regions	None	Regions to be used in the ensemble refinement
cif clean	yes, *positive integer*	Clean up the CIF file according to ELDICO and PDB
cif fit	default, none, high	Fit the CIF file according to the selected option
cif ref	auto	Use reference CIF file when a reference model is available
ignore chiral	None	Ignore the chirality in the SMILES string
ring-pucker-mode	None	Force rotamer in canonical 2d/3d/4d/5d
rotamer	yes, *positive integer*, "c-30", "c-60"	Rotamer rotamer rotamer to be used
maxcycle	*positive integer*	Run CIF optimization with this maximum number of cycles
tests	yes	Run CIF with this tests, if possible
ring-pucker	*positive integer*	Ring pucker to be used in a pucker
constraint-chiral	None	Constraint chiral
cutoff	None	Bond cutoff
cutoff-vdw	None	Cutoff for van der Waals
cutoff-hbond	None	Cutoff for hydrogen bonds
cutoff-vdw-h	None	Cutoff for van der Waals with hydrogen
cutoff-hbond-h	None	Cutoff for hydrogen bonds with hydrogen
hydrogens	"Algorithm determination", "True, False"	Hydrogens to be added to the ligand
ring-flip	None	Ring flip to be used in a pucker
ring-pucker-mode	None	Force rotamer in canonical 2d/3d/4d/5d

dlum_gui

Generating ligand structures and restraints in the eLBOW GUI

Overview

The electronic ligand Builder and Optimization Workbench (eLBOW) is the primary tool for generating non-standard chemical entities, in addition to providing geometry restraints for use in refinement. Typically, to the current source and source open, we compared with the phenix.ccp4 mon lib. In addition to eLBOW, a number of other programs are available for generating ligand structures and restraints, including Sketchers.

There are actually two eLBOW GUI available in the Cootbit menu. The first is a wizard-like interface that asks questions about the available inputs and the desired outcomes. The first screen asks for the basic inputs. These are analogous to the input options:

Above: The first screen of the wizard the eLBOW GUI with the Chemical component parameter selected

Once the basic inputs are provided the possible geometry optimizations are presented for selection:

Above: The second screen of the wizard the eLBOW GUI with the MM optimization parameter selected

Finally, the last screen is intended to show you the parameters that apply to your choices. You can make some more changes and run:

Above: Final screen of the wizard the eLBOW GUI

An advance GUI for expert or those who want to use some of the more complicated parameters is available.

Above: Main eLBOW Advanced Interface

Above: Other eLBOW Advanced Interface

Above: Other eLBOW Advanced Interface

Above: Other eLBOW Advanced Interface

Input files

eLBOW has extensive flexible options for describing ligand information. The only mandatory data are some description of the molecular topology, i.e. atomic connectivities and charges or explicit bond connectivity. Four main types of input information are:

- **SMILES string**. This is a compact syntax for uniquely representing molecules as text strings. Although it is not a standard, it is widely used and supported by many chemical software packages. It is usually the most reliable form of information to use, if available. You can also provide it as a file containing just the SMILES string.
- **Chemical file**. This is a file in the Mol2, Mol, or SDF file formats. Most of the time, the information in these files is sufficient to describe the molecular topology. Note that Mol2 files are also a type of input that is used by OMEGA toolkit, although OpenEye's OMEGA toolkit and the Schrödinger tool Jaguar.
- **Chemical Component Dictionary**. This is a file in the Chemical Component Dictionary format, or a Chemical Component Dictionary. Its definition is in the mmcif dictionary. Note that PDB's Ligand Expo provides a web interface to generate a CCD file for any ligand in the PDB. Note that the CCD is a superset of the information in the PDB's Chemical Component Dictionary, and that it is the main source of information for the Phenix.ccp4 mon lib.
- **PDB file**. This is a file in the PDB format. Although it is not a standard, it is widely used and supported by many chemical software packages. It is usually the most reliable form of information to use, if available. You can also provide it as a file containing just the PDB ATOM/HETATM records.

Output files

eLBOW can generate flexible options for describing ligand information. The only mandatory data are some description of the molecular topology, i.e. atomic connectivities and charges or explicit bond connectivity. Four main types of input information are:

- **SMILES string**. This is a compact syntax for uniquely representing molecules as text strings. Although it is not a standard, it is widely used and supported by many chemical software packages. It is usually the most reliable form of information to use, if available. You can also provide it as a file containing just the SMILES string.
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cell. If you are using a legal already present in the PDB and Grace the code, this is probably sufficient to get a good PDB file.
- **Generate Pdb**: this option will generate a PDB file based on the current Grace session.
- **Generate Pdb**: this option will generate the corresponding PDB file based on the current Grace session. This is useful if you want to edit the corresponding Grace session and save it to a new file, or if you want to generate a PDB file based on a Grace session that was created by a legal that is not present in the PDB. In the present case of ipsamilin, the PDB file does not necessarily need to be limited to the legal ipsamilin, but can also include other molecules such as solvent, ions, or other legals that are needed in the cell. The Grace sheet menu will automatically be populated with corresponding molecules.

Only one source of topology information may be provided but you may also provide the parameters for a additional legal. Grace will then combine the topology information of the two legals and write out a single PDB file. Grace does also allow adding new parameters for a legal at the same time when adding it to the file. Any parameter in the parameter file that is not present in the legal will be added to the PDB file.

A final source of information is a PDB file containing the template atom names, the geometry and topology information of the corresponding legal. Grace is not provided, Maxis will generate atom names for the output model and CIF file automatically.

Output files

The Maxis LEGAL-BF generates a PDB file and a CIF file, suitable for use in any other Maxis app (or third-party software). The output files are written to the directory specified in the Output Directory field in the Output Options dialog. These files also inherit information when legals such as Ligandbo, CarTopo, Grid-ligand and PDB file attributes (including ligand-level if you are dealing from a PDBX/mmcif file).

Above: the "Output ... / Legal ... / Legal ..."

Above: the "Output Options ... / Legal ...

What to do next

We recommend viewing the output CIF file (PDB) to make sure that the results are what you expect. The CIF file can be read into Maxis LEGAL-BF or any other software that supports the PDBx/mmCIF dictionary. Use the Ligandbo and Ligand2D extensions. If you have any details please your ligand in the model, the PDB file or the CIF file, you can use Maxis Ligand2D Drawing Ligand2D that is used in the.

References

1. **electronic Ligand Builder and Optimization Workbench (eLBOW) a tool for ligand coordinate and restraint generation**. Acta Crystallogr. D. Biol. Crystallogr. D. Biol. Crystallogr. 2010 Jan; 66(Pt 1):1-7. Epub 2009 Nov 20. PMC2.

Phenix *Python-based Hierarchical ENvironment for Integrated Xtallography*

Fitting a model into a cryo-EM map with em_placement

Author

1. Pavel Afonine (Pavel.Afonine@gmail.com)

Purpose

The em_placement tool docks the input model in a cryo-EM reconstruction, using the half maps in an adaptive reciprocal space way.

How em_placement works

The tool takes one component and performs a reference rigid and rotate shape or smooth functions in Fourier space. This information is used to predict whether or not a random search with a rotation model over the full reciprocal space is needed. If the search is needed, the tool performs a random search with a rotation model and the top ranking is selected to refine using target functions (see options below). Following this, translational search is performed using the same target function. The final model is then refined using real space refinement with optional rigid body options (selected or protein backbone) and a final cross-validation calculation.

The tool requires two half maps and a model. The model can be in any coordinate system and contain ligands.

Note: the statistical analysis requires the half maps to correspond to the full volume of the cryo-EM reconstruction. Using half maps from cryo-EM cannot be used.

Running em_placement

The tool can be run using command line arguments, but it can also be controlled by an input script using the gui option. A basic and simple script looks like the following, in which a model derived from the coordinate deposit of EMD-6224 is docked into the reconstruction of EMD-6224 deposit in EMDB entry 1ULB:

```
gui=False
remove_phasing_folder = True
model_1 = '''
CRYST1   98.000   98.000   98.000  90.00  90.00  90.00 P 4 3 2
SCALE1      0.010204  0.000000  0.000000        0.000000
SCALE2      0.000000  0.010204  0.000000        0.000000
SCALE3      0.000000  0.000000  0.010204        0.000000

ATOM      1  CA  ALA  A   1      -0.000  -0.000  -0.000  1.00 10.00           C
ATOM      2  CA  ALA  A   2      -0.000  -0.000   1.000  1.00 10.00           C
ATOM      3  CA  ALA  A   3      -0.000   1.000   1.000  1.00 10.00           C
ATOM      4  CA  ALA  A   4      -1.000   1.000   1.000  1.00 10.00           C
'''
```

If the pdb script is in a file named docking_script.pdb, the search would be run from the command line as:

```
phenix.real_space_refine docking_script.pdb
```

Most parameters specified in the script have been named in a way intended to convey the purpose of that parameter.

The output phasing folder parameter is provided in order to set the output directory produced by refinement, which is by default the current working directory. This is set to be deleted by the script above.

The gui=False group, commonly feature is only used at the moment to optionally generate a full assembly from a single chain.

The remaining composition parameter specifies the name of the containing the separation of all the components in the reconstruction.

The model 1 parameter is provided as an ungrouped search, which is normally recommended. Aspects of this search can be controlled with search and resources specified below. For example to limit to 24 GB search or to limit the search to 1 hour, the following command line options would be used:

```
phenix.real_space_refine docking_script.pdb resources.ram=24000 max_search_time=3600
```

Literature

- **Additional based signal and noise analysis for docking of models into cryo-EM maps**: P.V. Afonine, T. Terwilliger, A. Urzhumtsev, P.D. Adams. Acta Cryst. D (2021). 77, 1281-1291.
- **Cryo-EM model validation using phenix.real_space_refine**: P. Afonine, R.I. Poblet, T.G. Terwilliger, and P.D. Adams. Acta Cryst. D (2020). 76, 148-157.
- **Cryo-EM model validation using phenix.real_space_refine**: P. Afonine, R.I. Poblet, T.G. Terwilliger, and

List of all available keywords

AP_PATCHER
  - `patch_directory_to_dir` : [str] Replace the preceding folder path the dataspace of the end of the run
  - `input` : [str(dir) str(dir) numbers] Input directory
  - `dataset` : [str] Name of the dataset
                  the core is DEBRA FAST, not yet AP CORRECT CAN
  - **AP_CORE** :
    - `full_mpa` : [bool] Input full mpa file as alternative to half-maps
    - `half_mpa` : [bool] Input half-maps
    - `auto_prune_number` : [int] Initial number of pruned atoms from the PS, PS is an helical, default is 0 (no pruning)
    - `bond_constraint` : [bool] Bond constraint (applying a bond-length and a bond-angle of zero in the first cycle)
    - `soft_mask` : [bool] Relaxing mask by the soft-edge approximation found
    - `soft_mask_radius` : [int] Radius for the soft-edge approximation, default 10
                                   Radius for the soft-edge approximation, default 10
    - `fixed_positioning_mode` : [str] Fixed positioning mode, 'no' for no fixed positioning, 'yes' for fixed positioning, 'auto' for automatic fixed positioning
    - `fixed_positioning_step` : [int] Step for fixed positioning
                                   Step for fixed positioning
    - `varied_positioning` : [str(dir) str(dir)] Directory with varied positioning maps
    - **Image_Set_Variable** : Image selection variable
      - **Image_Set_Variable_Value** : Image selection variable value
    - **Cycle_Parameters** : Cycle parameters
      - `Cycle` : [int] Cycle
        - **Cycle_Variable** : Cycle variable
          - `Variable` : [str] Variable for the options for discarding correlation and ranking
          - **Cycle_Variable_Value** : Cycle variable value
            - `Cycle_Variable_Value` : [str] Cycle variable value for the options for discarding correlation and ranking
            - **Cycle_Variable_Value_Parameters** : Cycle variable value parameters
              - `Cycle_Variable_Value_Parameter` : [str] Cycle variable value parameter for the options for discarding correlation and ranking
  - **Ranking** :
    - `fit_processing` : [int] Fit processing, 1 for fit only, 2 for fit and ranking, 3 for ranking only
    - `fit_input_pkl` : [str] Fit input pkl for fit only or fit processing
    - `fit_output_pkl` : [str] Fit output pkl for fit only or fit processing
    - `ranking_input_pkl` : [str] Ranking input pkl for ranking only or fit processing
    - `refine_score` : [bool] Flag for whether or not to refine cc/ccc scores
    - `ccc` : [bool] Flag for whether or not to use ccc instead of cc for ranking and refinement
    - `map_top` : [int] Number of maps to be kept for further ranking in the cycle
                  Number of maps to be kept for further ranking in the cycle
    - `sym_axes_finder_n` : [int] Number of axes for the symmetry axes finder
    - `output_order` : [bool] Ordinal output for output files
    - `ccc_map_cut_off` : [int] Cut off value for ccc map, 0 for no cut off, 1 for average of half-maps
    - `ccc_map_cut_off_value` : [int] Cut off value, corresponds to sigma
                                [int] Cut off value, corresponds to sigma
    - **Cycle_Output** : Cycle output for all cycles
      - **Cycle_Output_Value** : Cycle output value
        - `Cycle` : [int] Cycle
        - `alpha` : [bool] Alpha for Euler rotation function angle
        - `beta` : [bool] Beta for Euler rotation function angle
        - `gamma` : [bool] Gamma for Euler rotation function angle
        - `shift` : [bool] Shift range for Euler rotation function
  - **Correlation_Level** :
    - **Correlation** :
      - `correlation_name` : [bool] Name
      - `weight_list` : [str] Weight list for the special model
      - `ccc_cut_off` : [int] Ccc cut off
      - `ranking_map_cutoff` : [int] Ranking map cutoff for top maps
    - **Network_Input** :
      - `network_input_name` : [str] Network input name
      - `fixed_weight` : [bool] Fixed weight for fixed model
      - `fixed_weight_file` : [str] Fixed model coordinates in .cmm or .cif
  - `out` : [str] Output directory
                  Out-specific parameter required for output directory

APMD Search for Increased Model Matching (AS) is the equivalent call to Fitch to supplemental and analytical information on a specific model. Unlike the Fitch Search, the APMD Search allows the user to specify a model and receive information on the closest matches, rather than just an exact match.

Usage and syntax for the APMD Search (AS) are almost identical to those of the Fitch Search.

```
$ ./apmd -d /usr/local/lib/fitch/data -m /usr/local/lib/fitch/models -AS -c /usr/local/lib/fitch/apmd.cfg
APMD Search
  -h, --help                  Show this help message and exit
  -V, --version               Show version and exit
  -m, --model-directory=DIRPATH
                              Directory where models reside
  -d, --data-directory=DIRPATH
                              Directory where data reside
  -c, --configuration=FILEPATH
                              Configuration file to use
  -o, --output=FILEPATH       Output file
  -v, --verbosity=LEVEL       Verbosity level (0 = quiet, 1 = normal, 2 = verbose)
  -S, --search=SEARCH         Search to perform

  Example: /bin/ls -AS -m /usr/local/lib/fitch -d /usr/local/lib/fitch -c /usr/local/lib/fitch/apmd.cfg
```

The APMD Search requires the same data and models files as the Fitch Search, plus a configuration file. The configuration file specifies naming rules based on geographicals, the amount value units, and the field analogous into account. The output is similar to the Fitch output, except shown below is the example FLEX output.

Unlike the Fitch Search, the APMD Search allows the user to specify a model and only one model and data is may be necessary to specify a different definition, e.g. `-m /usr/local/lib`.

The `-v` option controls verbosity level. Level 0 is quiet, level 1 is normal, and level 2 is verbose. Verbose output includes information about the search and the output. Quiet output includes only the output. Normal output includes the output and some information about the search and the output.

`/bin/ls -AS` controls an extraction search, such as contained in Fitch. Displays all possible matches. The search `-S` option allows the user to specify a search to perform. The search is a comma-separated list of search criteria. Each search criterion is of the form `field:value`. The `field` is the name of a field in the output. The `value` is the value to search for. If the value ends in `%`, it is treated as a wildcard. The `-o` option allows the user to write the output to a file instead of the default stdout.

Return to main interface.

Phonix Point Cloud Processing Framework for Integrated Workspaces

Docking a model into a local region of density with emplace_local

Authors

Kevin Ludwig, Claudia Pfeifer, Richa Chirlia, Thomas C Terwilliger

Purpose

The emplace_local tool docks the input model within a sphere of density centered on a defined point in the reconstructed density. This is useful for docking a trial molecular map and quality of fit statistics.

How emplace_local works

emplace_local takes a model and a density map. A local region of density is analyzed for local signal and cross-cluster of density in a sphere of specified radius. Optionally, a defined or a theoretical target for rotation and translation searches, which is used for scoring.

If half-maps are unavailable, just a full map can be provided and then the displayed target is defined by the density in the sphere centered on the specified center (default: cell).

The quality of fit can be scored by three factors:

1) average value of a cross correlation
2) the cross correlation of the model with local density (primary: CC)
3) the map correlation coefficient (CC for projected map CC) Darling

```
emplace_local
```

```
Keywords:
emplace_local docking fitting validation cryo-EM cryo-ET
emplace_local docking fitting validation cryo-EM cryo-ET
```

Note that the search center can be specified explicitly with the options center keyword (the usual approach) or with the keyword cell (default: cell) which uses the cell center (and providing a sphere center keyword).

It is also possible to provide a trial model as prior information.

Standard run of emplace_local

```
phenix.emplace_local model=model.pdb map=emdb_17138.map
phenix.emplace_local model=model.pdb map=emdb_17138.map
```

Literature

- **Conditional density-based and cross-analysis for docking of models into cryo-EM maps**, T.C. Terwilliger, P.V. Afonine, R.I. Read, and P.D. Adams. Acta Cryst. D79, 1-9 (2023) https://doi.org/10.1107/S2059798322010794
- **Phenix.emplace_local: Docking a model into a local region of density**, Kevin Ludwig, Claudia Pfeifer, Richa Chirlia, Thomas C. Terwilliger, and P.V. Afonine **in preparation**.
- **Phenix** Acta Cryst. D75, 861-877 (2019) https://doi.org/10.1107/S2059798319011471

List of all available keywords

```
model_file              Model file
map_file                Map file
sequence_file           Sequence file
sequence_combination    Optional sequence file and combination for full reconstruction,
                        Use this for full map calculation, the used if half-maps provided
map                     Map file for full map calculation, the used if half-maps provided
half                    Half map file if half map is provided
half2                   Half map file if half map is provided
mask                    Mask file
                        Optional mask file, used for calculation of half-map
                        correlation and for masking
optional_target         Optional target for docking
                        Optional target for docking
center                  Center
                        Optional explicit center (default cell)
cell                    Use cell center (default) or specified center
                        Use cell center (default) or specified center
initial_shift           Initial shift
                        Initial shift to apply to model
                        Initial shift to apply to model
search                  Search for optimal center
                        Search for optimal center
                        Search for optimal center
                        
```

phenix.ensemble_refinement

Purpose

phenix.ensemble_refinement is designed to combine X-ray structure refinement with molecular dynamics in order to generate ensembles of models that better represent the underlying crystal ensemble. Up to 128 individual structures and simultaneously account for anisotropy and anharmonic displacements.

phenix.ensemble_refinement is a command line tool that uses the Phenix and Cctbx libraries to perform molecular dynamics for ensemble refinement, X-ray crystallography, and refinement.

Simple test cases: Bucky-35, Bucky-2013, phenix.ensemble_refinement, a test study of apo and holo BACH1 transcriptional regulatory protein, and a test study of Lysozyme.

Application: Chandler & Terwilliger & Adams & Afonine & Afonine & phenix.ensemble_refinement: Benefits of ensemble refinement with anisotropy and anharmonicity. Acta Cryst D Vol. 77 Part 2 (2021)

General Procedure

The basic structure factor refinement workflow: refined single structure model (i.e. pdb phenix.refine, publication quality). If TLS is used the TLS components must be phased in the above model. (see phenix.tls). The optimal number of TLS groups is determined by the number of ensemble members and the resolution of the data.

Ensemble refinement workflow: refined single structure model (i.e. pdb phenix.refine, publication quality). If TLS is used the TLS components must be phased in the above model. (see phenix.tls).

For non-isotropic (particle-by-particle) refinement it is recommended to use harmonic restraints e.g.

phenix.ensemble_refinement model.pdb data.mtz harmonic_restraints=True harmonic_restraints_weight=1

Parameter Optimization

There are three main ensemble parameters that need to be optimized:

ptlevel=n

phenix.ensemble_refinement model.pdb data.ptlevel=2

This defines the number of atoms included in the TLS fitting procedure (see Berkley et al. 2010). This optimizes the number of TLS groups used in the ensemble refinement. Higher ptlevel values will result in more TLS groups and lower ptlevel values will result in fewer TLS groups. Default ptlevel=2 (3 TLS groups per chain) is the default setting. Ptlevel=1 (7 TLS groups per chain) is the most detailed setting.

ts phenix.ensemble_refinement model.pdb ts=50 data.ptlevel=2

This defines the number of ensemble members. Ts=50 is the default setting. Ts=128 is the maximum setting. Ensemble refinement with Ts=128 takes approximately 128 times longer than a single structure refinement. Ensemble refinement with Ts=50 takes approximately 50 times longer than a single structure refinement. Ts=1 is a single structure refinement.

ts phenix.ensemble_refinement model.pdb ts=50 ptlevel=2 data.mtz

Ensemble refinement with 50 ensemble members and 3 TLS groups per chain. Ensemble refinement with Ts=50 and ptlevel=2 takes approximately 150 times longer than a single structure refinement. Ensemble refinement with Ts=128 and ptlevel=1 takes approximately 896 times longer than a single structure refinement. Ensemble refinement with Ts=128 and ptlevel=2 takes approximately 384 times longer than a single structure refinement. Ensemble refinement with Ts=128 and ptlevel=3 takes approximately 128 times longer than a single structure refinement.

tx phenix.ensemble_refinement model.pdb tx=0.01 data.mtz

Temperature factor. Default tx=0.01 is the default setting. Tx=0.01 is a good value for most data. Tx=0.01 is the default setting. Tx=0.01 is a good value for most data. Tx=0.01 is the default setting. Tx=0.01 is a good value for most data.

phenix.ensemble_refinement model.pdb data.mtz

phenix.ensemble_refinement model.pdb data.mtz harmonic_restraints=True

phenix.ensemble_refinement model.pdb data.mtz harmonic_restraints=True harmonic_restraints_weight=1

phenix.ensemble_refinement model.pdb data.mtz harmonic_restraints=True ptlevel=2 ts=50 tx=0.01

phenix.ensemble_refinement model.pdb data.mtz ptlevel=2

phenix.ensemble_refinement model.pdb data.mtz ptlevel=2 ts=50

phenix.ensemble_refinement model.pdb data.mtz ptlevel=2 ts=50 tx=0.01

phenix.ensemble_refinement model.pdb data.mtz ptlevel=2 ts=50 tx=0.01 harmonic_restraints=True

phenix.ensemble_refinement model.pdb data.mtz ptlevel=2 ts=50 tx=0.01 harmonic_restraints=True harmonic_restraints_weight=1

The ensemble refinement tools have been set up to have as accessible many keywords as possible. Keywords that are not optimized or unused by base tools will if they be necessary to optimize the transformation tool offset parameters.

The tx=0.01 and tx=0.01 are only a rough reference for a typical ensemble refinement. Ensemble refinement at least at tx=0.01 and tx=0.01 is a good place to start. Ensemble refinement at tx=0.01 and tx=0.01 is a good place to start.

R-free values are also

```
  total_pot_limit : 0.75  # Total Total Potlimits bets BB potsize(0.50, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 11.0, 12.0, 13.0, 14.0, 15.0, 16.0, 17.0, 18.0, 19.0, 20.0, 21.0, 22.0, 23.0, 24.0, 25.0, 26.0, 27.0, 28.0, 29.0, 30.0, 31.0, 32.0, 33.0, 34.0, 35.0, 36.0, 37.0, 38.0, 39.0, 40.0,
```

Ensembler

Python based Hierarchical Mechanism for Sequence Multiplexing

Ensemble creation with Ensembler

Author(s)

J. Christopher Anderson
J. Christian Ibin, Nathanael Schaeu

Purpose

Ensembler can be used to supersede multiple chains to be used as an ensemble search model for molecular replacement.

See also

phenix.superior and phenix.ensembler have been superseded by phenix.super, ensembler.

Usage

Ensembler can be run from the PHENIX GUI and the command line, the only difference being the way coordinate files are specified.

The program uses multiple models of different protein chains as one of the main sources for frequently used ensembles. Ensembler can also use a single model and generate a set of ensembles from it. The program can be used as a step and then stop into the minimal state. The types are automatically recognized, and added to the ensemble automatically.

Input files

- **Structures** (mandatory): The chains that are to be superposed. Protein chains are automatically aligned, and nucleic acid chains are superposed based on the phosphate backbone. Ligands are not used.
- **Multiple sequence alignments** (MSA, Mandatory): Alignments of the chains to be superposed. Accepted formats are Clustal, Stockholm, and FASTA. Alignments are used to determine the sequence identity and coverage of the chains, and to be analyzed by phenix.ensembler and supplying alignment files. Ensembler extracts (with the corresponding chain) the sequence from the PDB header, or "UNKNOWN" and "UNKNOWN" are considered the same.

Output files

The superposed chains can be written out either as a pure multiple model PDB file that is readable by phenix.ensembler, or as individual files in a directory. The multiple model file is recommended because it keeps the alignment information with the structure. The individual files can be changed, but the alignment information will be lost (without phenix.ensembler).

Description

The workflow consists of several stages that can be independently configured. These are listed in order of operation, and can be run individually by specifying the stage name. The stages are: **sequence mapping**, **alignment mapping**, **weighting**, **superposition**, **clustering**, **sorting**, and **ensemble creation**.

Sequence mapping

Establishes the equivalence of residues among the input chains. There are several options available:

- **cut**: The default mode (with alignment mapping).
- **sequence**: Uses the sequence of the chain to determine the equivalence of residues.
- **alignment**: If set multiple multiple alignment is used, the alignment mapping will be used if this is specified (otherwise sequence mapping is used).
- **alignment**: Uses alignments to assign **all the same first sequence** (i.e. chains of homologous sequence are treated as identical). This is the default if multiple alignments are supplied, and is recommended for cases of ancient chains.
- **cut**: Cuts the alignment to sequence with insertion code left be used.

Post-sequence mapping mapping is quite a lot of the alignment can be done on this a improvise (e.g. no insertion codes, or cut to the sequence of the first chain).

Atom mapping

Maps equivalent atoms within equivalent residues to each other. The mapping is done by name hence the order of atoms in the residue does not matter. If atoms are missing from certain residues in a certain residue (minor side chain atoms, OXT, etc.) the mapping will be incomplete, and the superposition will be less accurate.

Superposition

Superposition of equivalent atoms. Ensembler is from a globally optimal solution. There are two superposition algorithms, Kabsch and Quaternion, which in turn have several options.

- **kabsch**: The superposition uses all equivalent atoms and gives equivalent weight to all equivalent atoms.
- **quaternion**: Uses the quaternion method to determine the superposition. Supports weighting and iterative clipping for clusters with outlier sequence identity. For the cluster algorithm, see Kabsch-Dodson 1992.

Both algorithms use Diamond's formulation to solve the pairwise relational superposition problem (Diamond 1990).

An exception is raised if there are less than 3 atoms present for superposition.

Ensembler supports iterative clipping of outlier residues based on the initial pairwise superposition. The convergence criteria are controlled by the cut parameter (if the maximum cut angle, which is the r.m.s. difference between the rotation matrix and identity).

Weighting

Automatic weighting can be used to improve superposition, either to amplify highly homologous regions or to decrease the effect of ancient one-sequence clusters (more because of a strong alignment). Implemented weighting schemes are:

- **cut**: cut weighing equivalent to no weighting.
- **density-decay**: Percent identical weighting scheme (default). This tends to converge first and give more weight to the conserved regions. Weight is given by:

$$w = \frac{1}{1 + \exp(-\frac{\text{identity} - 0.5}{\text{decay}})}$$

where w is the deviation from the average, Tolerance is an empirical value, and its optimal value is dependent on the sequence identity and decay is controlled by the cutoff parameter of the density-cutoff mode.

Weighting is blended with superposition with weights coverage, which can be controlled by the coverage-power parameter (default: 1.0).

In case of highly disparate structures (or ancient relative relatives), weight determination may temporarily be turned off by setting the cutoff parameter to 0.0. Alternatively, the weighting can be turned off by setting density-cutoff parameter of the weighing-scheme, with a lower value (controlled by the density-cutoff parameter, default: 0.5) and the weighting will be used if the superposition is good.

Cluster analysis

Hierarchical cluster analysis is performed using the pairwise r.m.s. differences as a distance measure. The hierarchical clustering algorithm and linkage method can be used to obtain cluster boundaries.

Chain Scissoring

The program trims residues from the final superposed model where the unweighted r.m.s.d. is above a certain threshold (default: 3.0 Å). This is controlled by the scissor-cutoff parameter. Scissoring flexible loops can, by default, be disabled.

Sorting

After superposition is complete, the chains can be sorted by sequence identity (sorting-function of sorting-mode), or by the weighted r.m.s.d. (default). The sorting function can be changed to RMSD (default). This is controlled by the sorting-mode parameter of the cluster stage. Default: read order (input).

Command line

```
phenix.ensembler
  [-h] [--version] [-v]
  [--verbose] [--quiet] [--debug]
  [--dry-run] [--stop-at-step=STEP]
  [--stop-after=STEP]
  [--output-dir=DIR]
  [--output-prefix=PREFIX]
  [--output-log=FILE]
  [--output-ensemble=FILE]
  [--output-chain=FILE]
  [--output-multiple=FILE]
  [--output-format=FORMAT]
  [--output-cut=FILE]
  [--output-weight=FILE]
  [--output-cluster=FILE]
  [--output-sorted=FILE]
  [--output-log-ensemble=FILE]
  [--output-log-chain=FILE]
  [--output-log-cut=FILE]
  [--output-log-weight=FILE]
  [--output-log-cluster=FILE]
  [--output-log-sorted=FILE]
  [--output-log-multiple=FILE]
  [--output-log-format=FORMAT]
  [--output-log-level=LEVEL]
  [--output-log-append]
  [--output-log-no-header]
  [--output-log-no-footer]
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  [--output-log-no-stdout-stderr-file-name-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix]
  [--output-log-no-stdout-stderr-file-name-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix]
  [--output-log-no-stdout-stderr-file-name-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix]
  [--output-log-no-stdout-stderr-file-name-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix]
  [--output-log-no-stdout-stderr-file-name-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix]
  [--output-log-no-stdout-stderr-file-name-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix]
  [--output-log-no-stdout-stderr-file-name-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix-suffix-prefix
```

Phenix

Python-based Hierarchical Environment for Integrated Xrystallography

Ensemble creation with Ensembler

Contents

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- Search for homologs for cluster prototypes
  - Structural superposition
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Purpose

Ensembling is a superposition of multiple homologous structures, which often gives superior performance when used in molecular replacement.

Usage

There is a standalone ensembler, one program available from the command line. The prefixed mode preparation phase of phenix.ensembler is available from the command line through the PHENIX GUI.

Input files

Input PDB files (required)
- Homologs (optional): The Ensembler pipeline can be bypassed, Ensembler/MMTBX/Phenix also implements homology searches. The clients that use the ensembler (phenix.ensembler) have options to specify a set of homologs to be used in place of those found by the ensembler. These options include options to whether those clients have the same chain(s). Homologs can also be transferred to the appropriate chain(s) in the ensemble, and the ensembler can optionally prune them based on sequence identity to the target sequence. Ensembler/MMTBX/Phenix also implements a variety of options for sequence alignment and structural superposition, and the ensembler can optionally prune the ensemble based on structural similarity. Finally, the ensembler can optionally perform a refinement step against the target structure. Supported formats: PDB. Recognized extensions: .pdb, .ent.
- Alignments (optional): Ensembler/MMTBX/Phenix can optionally use alignments provided by the user instead of those found by the ensembler. Alignments can be specified in a variety of formats, and the ensembler can also use alignments that are embedded in the input PDB files. Alignments can be used to specify which chains in the ensemble are homologs to which chains in the target, and to specify the target sequence corresponding to each ensemble chain. Alignments can also be used to specify the ensemble sequence, if the ensemble is not a subset of the target sequence. Supported formats: PIR, Clustal, Stockholm, HHpred, HHsearch, HHblits, HMMER, FASTA, PDB, PDBX/mmCIF, Phenix.

Output files

The ensemble chains can be written out either as a single multichain PDB file or as separate files. Alternatively, the ensemble can be written out as a single multichain PDB file with chains A and B in each chain, the phenix.ensembler keyword can be used (phenix.write_ensemble_pdb) to write out the ensemble in this format (if the PDB file has more than two chains, the ensemble will be written out as multiple files, one for each pair of chains, and the phenix.ensembler keyword will be ignored).

Description

The ensemble consists of several stages that can be independently configured. These are listed in order of operation. It is possible to run a preparation with the corresponding defaults, see the Command line section.

Model input

The ensemble phase has definition of structure assemblies in a flexible manner and is also backwards compatible with the previous version of ensembler (which assumed that there is one chain per structure).

Single-chain structures

These are inputs that are treated as if they are single chains and if there is more than one chain in a file, these are treated as if they were separate. Alternatively, if it is also possible to select participating chains in a multichain structure, see below.

For example, the sequence of chains A and B of chains A and B in the following PDB is needed (these are treated as separate chains):

```
CRYST1   52.000   52.000   52.000  90.00  90.00  90.00 P 1           1
ATOM      1  N   ASP A   4      -1.000   0.000   0.000  1.00 20.00           N
ATOM      2  CA  ASP A   4       0.000   0.000   0.000  1.00 20.00           C
ATOM      3  C   ASP A   4       1.000   0.000   0.000  1.00 20.00           C
ATOM      4  O   ASP A   4       2.000   0.000   0.000  1.00 20.00           O
ATOM      5  N   ASP B   4      -1.000   1.000   0.000  1.00 20.00           N
ATOM      6  CA  ASP B   4       0.000   1.000   0.000  1.00 20.00           C
ATOM      7  C   ASP B   4       1.000   1.000   0.000  1.00 20.00           C
ATOM      8  O   ASP B   4       2.000   1.000   0.000  1.00 20.00           O
```

Multimeric assemblies

In this case the individual assemblies need to be specified along either the source keyword or through the phenix.ensembler keyword (phenix.ensembler.source). Assemblies are specified by a comma-separated list of chains.

In case the input PDB file contains multiple PDBXs/mmCIFs, assemblies can be specified by comma-separated assemblies and the further selection is required. Assemblies are specified by chain IDs from the assembly1 (for example, if there are chains A and B in the assembly1 and C and D in the assembly2, the chain IDs are A and C).

For example, if there are two assemblies in a structure, the first one consisting of chains A and B and the second one consisting of chains C and D, the following command line will create a dimer and a tetramer:

```
phenix.ensembler source=A,C
```

To specifically select the assemblies, the following input is required:

```
phenix.ensembler
  input {
    file_name = "/path/to/file.pdb"
    assembly = "1,2"
    assembly = "1,3"
  }
```

To specifically select the chains A and B in the assembly1 and C and D in the assembly2, the following input is required:

```
phenix.ensembler
  input {
    file_name = "/path/to/file.pdb"
    assembly = "A,B"
    assembly = "C,D"
  }
```

Multiple sequence alignments

Multiple sequence alignments can be specified using the alignment keyword (phenix.ensembler.alignment). Alignments are specified by a comma-separated list of alignments and the alignment keyword can also be used to specify the target sequence. Alignments can also be specified in a variety of formats and the ensembler will attempt to read them in a variety of formats.

For example, to request non-default mapping options for the 4ZYI example, the following options are needed (the target is requested for demonstration):

```
phenix.ensembler
  input {
    file_name = "/path/to/file.pdb"
    assembly = "A,B"
    assembly = "C,D"
    alignment = "/path/to/file.hhsearch"
    target = "/path/to/file.fasta"
  }
```

The pdb and the two alignments (chains A and B) and (chains C and D) are for the chains A and B and C and D in the chain A and in Note that these provide and the defaults for chains A and B (assembly1 (chains A and B)) and C and D (assembly2 (chains C and D)). Alternatively, the alignments can be specified in a way that allows the ensembler to find the appropriate alignment for each chain, for example:

```
phenix.ensembler
  input {
    file_name = "/path/to/file.pdb"
    assembly = "A,B"
    assembly = "C,D"
    alignment = "/path/to/file.hhsearch"
    alignment = "/path/to/file.hhsearch"
    target = "/path/to/file.fasta"
  }
```

In this case, alignments for specific mapping is requested for assembly positions (chains A and B, the default options will be used).

Atom mapping

Maps selected atoms within equivalent residues to each other. The mapping is done by name hence the order of atoms in the residue does not matter. The mapping is used in the superposition and in the refinement step.

Atom selection is controlled by the atom parameter of the superposition scope. If multiple atom names are specified, the ensembler will attempt to map the first atom in the list, if it is not present in the residue, it will attempt to map the second atom in the list, and so on. If the atom is not present in any of the specified atoms, there will be no atom mapping for that residue.

For example, if the ensembler is to prune based on alpha-carbon and use alpha-carbon for superposition, the following input is required (the target is requested for demonstration):

```
phenix.ensembler
  input {
    file_name = "/path/to/file.pdb"
    assembly = "A,B"
    assembly = "C,D"
    alignment = "/path/to/file.hhsearch"
    alignment = "/path/to/file.hhsearch"
    target = "/path/to/file.fasta"
  }
  superposition {
    atom = "CA"
  }
  prune {
    atom = "CA"
    method = "rmsd"
    cutoff = 1.5
    reference = "C"
    keep = 10
  }
```

The pdb and the two alignments (chains A and B) and (chains C and D) are for the chains A and B and C and D in the chain A and in Note that these provide and the defaults for chains A and B (assembly1 (chains A and B)) and C and D (assembly2 (chains C and D)). Alternatively, the alignments can be specified in a way that allows the ensembler to find the appropriate alignment for each chain, for example:

```
phenix.ensembler
  input {
    file_name = "/path/to/file.pdb"
    assembly = "A,B"
    assembly = "C,D"
    alignment = "/path/to/file.hhsearch"
    alignment = "/path/to/file.hhsearch"
    target = "/path/to/file.fasta"
  }
  superposition {
    atom = "CA"
  }
  prune {
    atom = "CA"
    method = "rmsd"
    cutoff = 1.5
    reference = "C"
    keep = 10
```

Explore Metric Symmetry

Purpose

phenix.explore_metric_symmetry is a program that allows a user to quickly determine the symmetry of the lattice, point group, and, and determine relations between various possible point groups.

Another use of phenix.explore_metric_symmetry is in the comparison of related unit cells, that are related by a change of basis or a change of lattice identity.

Keywords

A list of keywords and similar help can be obtained by typing: phenix.explore_metric_symmetry

```
  help=keywords
  keywords=[keyword1,keyword2,...]
  keyword=all                 Show this help message and exit
  keyword=cell                Input unit cell parameters
  keyword=group               Input point group
  keyword=lattice             Input lattice identity
  keyword=cell_tolerance      Relative cell tolerance for comparisons
  keyword=angle_tolerance     Angular tolerance for comparisons (deg)
  keyword=lattice_tolerance   Relative cell tolerance for lattice identification
                              Default: 0.0(0 disabled)
  keyword=lattice_id          Output lattice identity
  keyword=point_group         Output point group (or output the point group
                              given if specified with keyword=group)
  keyword=NONE                Output all possible point groups
                              (if lattice identified and point group not given)
                              Default: output point group(s) for the input cell
  keyword=reg_tolerance       Relative tolerance for regularization
                              Default: 0.05
  keyword=reg_type            Type of regularization, choose from R,A,B,C,I,F
                              Default: R (reduced)
  keyword=point_group_output  Output point group(s) for unit cell comparison
                              (if point group not given)
                              Default: output point group(s) for unit cell
                              comparison
  keyword=point_group_tolerance Point group tolerance
                              Default: 0.05
  keyword=point_group_type    Point group type, choose from P,A,B,C,I,F
                              Default: P
  keyword=cell_tolerance      Relative cell tolerance for unit cell comparisons
                              Default: 0.05
  keyword=angle_tolerance     Angular tolerance for unit cell comparisons
                              Default: 5.0 (deg)
  keyword=cell_type           Type of unit cell, choose from P,A,B,C,I,F
  keyword=cell_tolerance      Relative tolerance for unit cell type
                              Default: 0.05
  keyword=angle_tolerance     Angular tolerance for unit cell type
```

Python-based Hierarchical ENvironment for Integrated Xtallography

phenix.f000: gives F000 fix and cases bulk-solvent density estimate F000 reflection

Description

This program reads PDB model and optionally provided mask bulk-solvent density value (default is 0.35e/A^3)

Output: estimate of F000 value and solvent content

Command line usage examples

```
phenix.f000 model.pdb
phenix.f000 model.pdb mask_solvent_density=0.40
```

fab_elbow_angle

Phenix *Python-based Macromolecular Refinement for Enhanced Crystallography*

Calculating Fragment Antigen-Binding (Fab) elbow angle

Overview

Fab (Fragment Antigen-Binding) consists of two parts, the light chain (variable domain VL and constant CL) and the heavy chain (variable domain VH and constant domain CH1). The angle between the variable and constant domains in the Fab elbow region is important for antibody function and stability. The program fab_elbow_angle calculates the elbow angle between the VL and VH domains, using the standard Fab elbow definition by aligning the light portion of each structure, to the heavy one.

Command line options:

- **pdb** PDB file name (required, no default set to).
- **heavy** chain ID of heavy domain (no default set to).
- **light** chain ID of light domain (no default set to). Variable and constant domains in the light chain, by default 1C1.
- **shift** shift in number of the residue separating between variable and constant domains in the heavy chain, by default 113.
- **-h** help

Usage:

```
cctbx.fab_elbow_angle fab_name.pdb light=L1 heavy=H1 [limit_n=1257] [shift_h=113]
```

Examples:

```
cctbx.fab_elbow_angle 7fab.pdb light=L heavy=H limit_n=108 limit_h=127
```

```
cctbx.fab_elbow_angle 1fdl.pdb
```

```
cctbx.fab_elbow_angle 1fdl2.pdb
```

```
cctbx.fab
```

phenix.fem: compute Feature Enhanced Map (FEM)

Reflection Oriented Maximum Likelihood for Enhanced Cryoscopy

Description

The program uses PDB model, reflection data (Fobs or data), experimental uncertainties and R-free flags to compute Feature Enhanced Map (FEM) and Maximum Likelihood Weighted Difference Map (DFMC) as described in:

Frederick A Vallese, Oleg Fischer, Vincent Chen, Jeffrey Mendez, Peter Berkowitz, Oleg Fischer, Nicholas Sauter, Oleg Fischer, Cryo-EM Feature Enhanced Maps: Identification of Ligand Binding Sites and Protein Structure Refinement, bioRxiv 2022.02.14.480415; doi: https://doi.org/10.1101/2022.02.14.480415 [preprint]

Frederick A Vallese, Oleg Fischer, Vincent Chen, Jeffrey Mendez, Peter Berkowitz, Oleg Fischer, Nicholas Sauter, Oleg Fischer, Cryo-EM Feature Enhanced Maps: Identification of Ligand Binding Sites and Protein Structure Refinement, Structural Dynamics 10, 014101 (2023); https://doi.org/10.1063/4.0000205 [publication]

Oleg Fischer, Nicholas Sauter, Oleg Fischer, Feature Enhanced Cryo-EM Maps and Maximum Likelihood Weighted Difference Maps, Acta Cryst. A79, 1-8 (2023); https://doi.org/10.1107/S2053273322010835 [publication]

Oleg Fischer, Nicholas Sauter, Oleg Fischer, Feature Enhanced Cryo-EM Maps and Maximum Likelihood Weighted Difference Maps, Acta Cryst. A79, 1-8 (2023); https://doi.org/10.1107/S2053273322010835 [publication]

Program uses PDB model, reflection data (Fobs or data), experimental uncertainties and R-free flags to compute Feature Enhanced Map (FEM) and Maximum Likelihood Weighted Difference Map (DFMC) as described in PDB

Program uses the same phase error of Fourier coeff-ficients, namely:

- pcalcfom,dfmcfom(phi, weight,CorrMap,CRFomapc,fMapc,scale): signal a congruent
- CorrMap,CRFomapc,fMapc,scale: Correlation Map, Cross-R-factor Map, Feature Map, scale factor
- CRFomapc=(Fobs-scale*fMapc)/Fobs: Cross-R-factor Map
- CorrMap=sqrt(1-CRFomapc*CRFomapc): Correlation Map

Command line usage examples:

1. Specify data and model:
   - phenix.fem data=1ubq.mtz model=1ubq.pdb
2. Specify data label:
   - phenix.fem data=1ubq.mtz model=1ubq.pdb labels=fobs
3. Specify scattering dictionary (if neg. electrons, neutron):
   - phenix.fem data=1ubq.mtz model=1ubq.pdb scattering_table=neutron
4. Score other settings and their defaults:
   - phenix.fem data=1ubq.mtz model=1ubq.pdb
   - use_fmodel=true: use fmodel FM as data fmap
   - use_fmodel=false: use data fmap (default)
   - fem_name=phenix.fem: map prefix for output
   - fem_cycle=1: number of FEM cycles (only one supported in the command line)

GUI

Graphical user interface is available.

Additional information:

Latest documentation of FEM methodology:

https://phenix.sourceforge.net/mailinglists/fem_SBMB2022.pdf

Publication in Computational Crystallographic Newsletter (front page):

http://www.phenix-online.org/newsletter/CCN_2022_07.pdf

References

- **Frederick A Vallese, Oleg Fischer** Vincent Chen, Jeffrey Mendez, Peter Berkowitz, Oleg Fischer, Nicholas Sauter, Cryo-EM Feature Enhanced Maps: Identification of Ligand Binding Sites and Protein Structure Refinement, bioRxiv 2022.02.14.480415; doi: https://doi.org/10.1101/2022.02.14.480415 [preprint]
- **Oleg Fischer**, Cryo-EM Feature Enhanced Maps, Structural Dynamics 10, 014101 (2023); https://doi.org/10.1063/4.0000205 [publication]
- **Oleg Fischer**, Feature Enhanced Cryo-EM Maps and Maximum Likelihood Weighted Difference Maps, Acta Cryst. A79, 1-8 (2023); https://doi.org/10.1107/S2053273322010835 [publication]

List of all available keywords

```
model_name = None
use_mtrff = True                    Use remote MTZ protocol
  .type = bool
use_pcalcfom = True
  .type = bool
signal_threshold = 0.5
  .type = double
use_dfmc_map = True
  .type = bool
labels_data_accepted_phases = True
  .type = bool
input
  .phenix = True
  .help = Input to phenix CCP4MG PO phenixscript Material interface.
  wavelength = None
  .type = double
  use_input_model_phases = True
  .type = bool
  file_name = None                  Files of X-ray data and free-R flags
    .type = path
    .multi = True
    .output = False
    .gui = True
    .wizard = True
    .style = file_type:hkl,file_type:mtz
    .help = Reflection data, either mtz(mtz) or hkl(shelx format)
    .short_caption = Reflection data
  fmodel_phase_source = True
  .type = bool
  scale_fmodel_scattering_principle = None
  .type = choice(multi=False)
  .help = Scale fmodel to data using Wilson scaling or by matching total scattering
  labels = None
    .type = str
    .multi = True
    .help = Data labels (for example, FOBS,SIGFOBS)
    .short_caption = Data labels
  convert_to_mm_anomalous_if_data_parts_have_both_friedel = False
  .type = bool
  fmodel
    .type = str                     Minimum number of functional tests
    .help = Minimum number of reflections per bin
    .short_caption = Minimum number of reflections per bin
    .expert_level = 1
    .multi = False
    .gui = True
    .wizard = True
    .style = bold
    .help = Specify if fmodel fmap will be used as possible (or else pseudonym)
    .short_caption = Use fmodel
    .allow_multiple_selections = False
    .value_at_least = 0.0
    .value_at_most = 1.0
    .step = 0.1
    .allow_auto = False
    .allow_none = False
    .allow_all = False
    .allow_random = False
    .allow_unique = False
    .allow_all_but_one = False
    .allow_all_but_two = False
    .allow_all_but_three = False
    .allow_all_but_four = False
    .allow_all_but_five = False
    .allow_all_but_six = False
    .allow_all_but_seven = False
    .allow_all_but_eight = False
    .allow_all_but_nine = False
    .allow_all_but_ten = False
    .allow_all_but_eleven = False
    .allow_all_but_twelve = False
    .allow_all_but_thirteen = False
    .allow_all_but_fourteen = False
    .allow_all_but_fifteen = False
    .allow_all_but_sixteen = False
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    .allow_all_but_twenty_twenty_twenty_eight = False
    .allow_all_but_twenty_twenty_twenty_nine = False
    .allow_all_but_twenty_twenty_twenty_ten = False
    .allow_all_but_twenty_twenty_twenty_eleven = False
    .allow_all_but_twenty_twenty_twenty_twelve = False
    .allow_all_but_twenty_twenty_twenty_thirteen = False
    .allow_all_but_twenty_twenty_twenty_fourteen = False
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    .allow_all_but_twenty_twenty_twenty_sixteen = False
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    .allow_all_but_twenty_twenty_twenty_twenty = False
    .allow_all_but_twenty_twenty_twenty_twenty_one = False
    .allow_all_but_twenty_twenty_twenty_twenty_two = False
    .allow_all_but_twenty_twenty_twenty_twenty_three = False
    .allow_all_but_twenty_twenty_twenty_twenty_four = False
    .allow_all_but_twenty_twenty_twenty_twenty_five = False
    .allow_all_but_twenty_twenty_twenty_twenty_six = False
    .allow_all_but_twenty_twenty_twenty_twenty_seven = False
    .allow_all_but_twenty_twenty_twenty_twenty_eight = False
    .allow_all_but_twenty_twenty_twenty_twenty_nine = False
    .allow_all_but_twenty_twenty_twenty_twenty_ten = False
    .allow_all_but_twenty_twenty_twenty_twenty_eleven = False
    .allow_all_but_twenty_twenty_twenty_twenty_twelve = False
    .allow_all_but_twenty_twenty_twenty_twenty_thirteen = False
    .allow_all_but_twenty_twenty_twenty_twenty_fourteen = False
    .allow_all_but_twenty_twenty_twenty_twenty_fifteen = False
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    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_fourteen = False
    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_fifteen = False
    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_sixteen = False
    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_seventeen = False
    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_eighteen = False
    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_nineteen = False
    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty = False
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    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_four = False
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    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_six = False
    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_seven = False
    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_eight = False
    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_nine = False
    .allow_all_but_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_twenty_ten = False
    .allow_all_but_twenty_tw
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phenix.find_all_ligands

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Finding all ligands in a map with phenix.find_all_ligands

Author(s)

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Purpose

phenix.find_all_ligands is a command line tool for finding all the ligands in a map by sequentially running phenix.ccp4cm (CCP4 suite of ligands) and choosing the best fitting one at each site.

Usage

How phenix.find_all_ligands works:

phenix.find_all_ligands runs the phenix.find_ligand procedure twice. The first is to identify the largest contiguous region of density in your map that is not already occupied by your model or previously fitted ligands. The second time it runs phenix.find_ligand with the specified region of interest. This time it will try to fit all ligands in the region. Any ligands fitting better than the best fitting ligand are deleted from consideration and the process is repeated until no more ligands are found. The output is a PDB file containing all the ligands found in the map.

Output files from phenix.find_all_ligands

The output files from phenix.find_all_ligands are similar to those from phenix.find_ligand. Differences include: ccp4cm.pdb.1 files will be files with names such as "ccp4_1_ATP.pdb" for the placement of ATP in the first ligand.

Examples

Standard run of phenix.find_all_ligands:

Running phenix.find_all_ligands is very simple, you will need a map in ccp4 or phenix format, a sequence file, and a model file. The following example shows the command line for running phenix.find_all_ligands. Timing and the first set of ligands commands detailed what exactly are being done:

```
phenix.find_all_ligands map.ccp4 seq.seq model.pdb
Starting ccp4cm ...
  ccp4cm -m map.ccp4 -s seq.seq -p model.pdb
  ccp4cm -m map.ccp4 -s seq.seq -p model.pdb
  ccp4cm -m map.ccp4 -s seq.seq -p model.pdb
  ccp4cm -m map.ccp4 -s seq.seq -p model.pdb
Ligands:
  ccp4_1_ATP.pdb
  ccp4_2_ADP.pdb
  ccp4_3_ATP.pdb
  ccp4_4_ADP.pdb
Ligands:
  ccp4_1_ATP.pdb
  ccp4_2_ADP.pdb
  ccp4_3_ATP.pdb
  ccp4_4_ADP.pdb
Ligands found: 4
Ligands found: 4
Ligands found: 4
```

search_parameters	
`tagged_with` : Tag	Tags to search for.
`tagged_with_all` : Tag	Tags that must be attached to all posts in order to be returned.
`tagged_with_exclusive` : Tag	Tags that must be attached to all posts in order to be returned, but not any other tags.
`tagged_with_all` : Tag	Tags that must be attached to all posts in order to be returned.
`group_search` : Bool	Set to true to search for groups instead of posts. Defaults to false.
`tagged_in_or` : Tag	Tags that must be attached to at least one of the tags in the tag list.
`tagged_exclusively` : Bool	Set to true to search for posts that are tagged only with the tags in the tag list.
`text_search` : String	Search for posts containing the tagged text.
`sort` : Sort	Sort the results by the specified criterion.
`page` : Int	Which page of results to return.
`only_in_blog` : Bool	Set to true to search only posts in the blog specified by the blog_id parameter.
`blog_id` : Int	Search posts in the blog with the specified ID.
`tagged_from_blog` : Int	Search for posts tagged with tags that are used in the blog specified by this blog ID.
`has_tagged_from_blog` : Bool	Set to true to only return posts that have tags that are used in the blog specified by the blog_id parameter.
`is_tagged` : Bool	Set to true to only return posts that are tagged.
`is_untagged` : Bool	Set to true to only return posts that are not tagged.
`is_photo` : Bool	Set to true to only return photo posts.
`is_text` : Bool	Set to true to only return text posts.
`is_quote` : Bool	Set to true to only return quote posts.
`is_link` : Bool	Set to true to only return link posts.
`is_video` : Bool	Set to true to only return video posts.
`is_audio` : Bool	Set to true to only return audio posts.
`is_answer` : Bool	Set to true to only return answer posts.
`is_reblog` : Bool	Set to true to only return reblog posts.
`is_liked` : Bool	Set to true to only return posts you have liked.
`is_following` : Bool	Set to true to only return posts from blogs you are following.
`is_private` : Bool	Set to true to only return private posts.
`is_mine` : Bool	Set to true to only return posts from your own blog.
`is_recommended` : Bool	Set to true to only return posts that are recommended by Tumblr.
`is_recommended_by_friends` : Bool	Set to true to only return posts that are recommended by Tumblr because your friends like them.
`is_recommended_by_you` : Bool	Set to true to only return posts that are recommended by Tumblr because you like similar posts.
`is_liveblog` : Bool	Set to true to only return liveblog posts.
`is_pinned` : Bool	Set to true to only return pinned posts.
`is_seen` : Bool	Set to true to only return seen posts.
`is_pending` : Bool	Set to true to only return pending posts.
`is_draft` : Bool	Set to true to only return draft posts.
`is_queued` : Bool	Set to true to only return queued posts.
`is_submission` : Bool	Set to true to only return submission posts.
`is_anonymous` : Bool	Set to true to only return anonymous posts.
`is_blocks_post` : Bool	Set to true to only return blocks post.
`is_blocked` : Bool	Set to true to only return blocked posts.
`is_unblocked` : Bool	Set to true to only return unblocked posts.
`is_unlocked` : Bool	Set to true to only return unlocked posts.
`is_locked` : Bool	Set to true to only return locked posts.
`is_unsent` : Bool	Set to true to only return unsent posts.
`is_unscheduled` : Bool	Set to true to only return unscheduled posts.
`is_scheduled` : Bool	Set to true to only return scheduled posts.
`is_unpublished` : Bool	Set to true to only return unpublished posts.
`is_unreviewed` : Bool	Set to true to only return unreviewed posts.
`is_reviewed` : Bool	Set to true to only return reviewed posts.
`is_rejected` : Bool	Set to true to only return rejected posts.
`is_unrejected` : Bool	Set to true to only return unrejected posts.
`is_ignored` : Bool	Set to true to only return ignored posts.
`is_unignored` : Bool	Set to true to only return unignored posts.
`is_reported` : Bool	Set to true to only return reported posts.
`is_unreported` : Bool	Set to true to only return unreported posts.
`is_flagged` : Bool	Set to true to only return flagged posts.
`is_unflagged` : Bool	Set to true to only return unflagged posts.
`is_spam` : Bool	Set to true to only return spam posts.
`is_unspam` : Bool	Set to true to only return unspam posts.
`is_trash` : Bool	Set to true to only return trash posts.
`is_untrash` : Bool	Set to true to only return untrash posts.
`is_ask` : Bool	Set to true to only return ask posts.
`is_unanswered` : Bool	Set to true to only return unanswered posts.
`is_unlimited` : Bool	Set to true to only return unlimited posts.
`is_limited` : Bool	Set to true to only return limited posts.
`is_unsupported` : Bool	Set to true to only return unsupported posts.
`is_supported` : Bool	Set to true to only return supported posts.
`is_unsupported_ios` : Bool	Set to true to only return unsupported iOS posts.
`is_supported_ios` : Bool	Set to true to only return supported iOS posts.
`is_unsupported_android` : Bool	Set to true to only return unsupported Android posts.
`is_supported_android` : Bool	Set to true to only return supported Android posts.
`is_unsupported_web` : Bool	Set to true to only return unsupported web posts.
`is_supported_web` : Bool	Set to true to only return supported web posts.
`is_unsupported_mobile` : Bool	Set to true to only return unsupported mobile posts.
`is_supported_mobile` : Bool	Set to true to only return supported mobile posts.
`is_unsupported_desktop` : Bool	Set to true to only return unsupported desktop posts.
`is_supported_desktop` : Bool	Set to true to only return supported desktop posts.
`is_unsupported_ipad` : Bool	Set to true to only return unsupported iPad posts.
`is_supported_ipad` : Bool	Set to true to only return supported iPad posts.
`is_unsupported_iphone` : Bool	Set to true to only return unsupported iPhone posts.
`is_supported_iphone` : Bool	Set to true to only return supported iPhone posts.
`is_unsupported_ipod` : Bool	Set to true to only return unsupported iPod posts.
`is_supported_ipod` : Bool	Set to true to only return supported iPod posts.
`is_unsupported_android_app` : Bool	Set to true to only return unsupported Android app posts.
`is_supported_android_app` : Bool	Set to true to only return supported Android app posts.
`is_unsupported_ios_app` : Bool	Set to true to only return unsupported iOS app posts.
`is_supported_ios_app` : Bool	Set to true to only return supported iOS app posts.
`is_unsupported_web_app` : Bool	Set to true to only return unsupported web app posts.
`is_supported_web_app` : Bool	Set to true to only return supported web app posts.
`is_unsupported_mobile_app` : Bool	Set to true to only return unsupported mobile app posts.
`is_supported_mobile_app` : Bool	Set to true to only return supported mobile app posts.
`is_unsupported_desktop_app` : Bool	Set to true to only return unsupported desktop app posts.
`is_supported_desktop_app` : Bool	Set to true to only return supported desktop app posts.
`is_unsupported_ipad_app` : Bool	Set to true to only return unsupported iPad app posts.
`is_supported_ipad_app` : Bool	Set to true to only return supported iPad app posts.
`is_unsupported_iphone_app` : Bool	Set to true to only return unsupported iPhone app posts.
`is_supported_iphone_app` : Bool	Set to true to only return supported iPhone app posts.
`is_unsupported_ipod_app` : Bool	Set to true to only return unsupported iPod app posts.
`is_supported_ipod_app` : Bool	Set to true to only return supported iPod app posts.
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`is_unsupported_iphone_app_ios` : Bool	Set to true to only return unsupported iPhone app iOS posts.
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find_all_orig_sym_mols:

phenix.find_all_orig_sym_mols: Identify equivalent MR solutions of the same dataset irrespective of origin and symmetry operation

Contents

- Author(s)
- Purpose
- Usage
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- Output to screen
- Do the MR solutions match?
- Keywords
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- Licensing
- Acknowledgements
- Cite us
- Comments/suggestions welcomed

Author(s)

- Pavel Afonine, Nigel Jones, Kevin D. Cowtan
- Paul D. Adams

Purpose

phenix.find_all_orig_sym_mols (or phenix.fasym) attempts to find the best superposition of two different molecular models (MR solutions) by trying all possible combinations of the two models' unit cell origins and symmetry operations and alternate-origin shifts permitted for the space-group of the crystal. Instead of using the phase information, it uses the atom coordinates. The two models can be obtained from two different MR runs or even one solution and a cryo-EM map. Results can be exported for all specific symmetry operations and alternate-origin shifts or just for the best one. The output can be used as input for other programs, for example, phenix.refine. This is designed for that particular job (it does).

Usage

phenix.find_all_orig_sym_mols (or phenix.fasym) [**find_alternate_origin_symmetry_mates** | **output_single** | **n_cycles** | **map_resolution** | **n_max** | **n_min** | **n_max_mols** | **n_min_mols** | **n_max_mols_per_asu** | **n_min_mols_per_asu** | **n_max_mols_per_cell** | **n_min_mols_per_cell** | **n_max_mols_per_sym** | **n_min_mols_per_sym** | **n_max_mols_per_sym_per_asu** | **n_min_mols_per_sym_per_asu** | **n_max_mols_per_sym_per_cell** | **n_min_mols_per_sym_per_cell** | **n_max_mols_per_sym_per_sym** | **n_min_mols_per_sym_per_sym** | **n_max_mols_per_sym_per_sym_per_asu** | **n_min_mols_per_sym_per_sym_per_asu** | **n_max_mols_per_sym_per_sym_per_cell** | **n_min_mols_per_sym_per_sym_per_cell** | **n_max_mols_per_sym_per_sym_per_sym** | **n_min_mols_per_sym_per_sym_per_sym** | **n_max_mols_per_sym_per_sym_per_sym_per_asu** | **n_min_mols_per_sym_per_sym_per_sym_per_asu** | **n_max_mols_per_sym_per_sym_per_sym_per_cell** | 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**n_min_mols_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym** | **n_max_mols_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_asu** | **n_min_mols_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_asu** | **n_max_mols_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_cell** | **n_min_mols_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_cell** | **n_max_mols_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym_per_sym** | **n_min_mols_per_sym

Fig. 1

In the case illustrated above the chains A, B, C in the 3Rx.cif pdb set have unique pairwise matching with chains D, E, F in the 4Ax.cif pdb set. The A chain is the top file in both pdb sets and pairwise matching with the D chain. The pair of chains B and E is the second pair in the 3Rx.cif and 4Ax.cif pdb sets. The pairwise matching of the C and F chains is the last of the big file (where the RMSDs of the pairs of matched chains. Even the results tab the superposed structures are shown. Below the Log output, Log output, Superposed and the RMSD matrix of the superposed pdb structures.

Open in Coot
Open in PyMOL
Open in Mol*
Open Superposed Structures
Open Superposed Structures
Open Superposed Structures

find_helices_strands

Python Issues Resolved Phenomenal for Integrated Bioinformatics

Rapid fitting of secondary structure in a map with find_helices_strands

Contents

- Author(s)
- Purpose
- Success the process
- Syntax
- Input and output records in template phenix.autobuild
- Complete Manual
- Tips and hints for new problems
- References
- List of available keywords

Author(s)

- Tom Ioerger, strands, Tom Terwilliger
- Author: Tom Ioerger

Purpose

The Strands program is a program that uses for finding helices and strands in a map and helices as model of the

parts of a structure that have regular secondary structure. It can be used to predict, dock, and DEEP, for alpha helices, beta strands, and alpha helices and beta strands. It can also be used to predict, dock, and DEEP, for alpha helices and beta strands.

Running the program

The program is available in the Rosetta GUI under "Rosetta Scripting". The only required input is an electron density map, such as the output of density modification. A protein sequence is optional.

Scattering and Density Search job qsub
Job Distribution
Job Inputs
Job Outputs
Job Options
Input Jobs
Input Jobs
Input Jobs

Phenix

Action-based Hierarchical Environment for Integrated Crystallography

Finding and analyzing NCS from heavy-atom sites or a model with find_ncs

Contents

- Authors
- Purpose
- Standard run of find_ncs
- Creating a model containing solvent sites
- Output files from find_ncs
- Format of NCS operators
- Format of NCS definitions
- Keywords
- Standard run of find_ncs
- Creating a model containing solvent sites
- Additional information
- References
- List of all available keywords

Authors:

- Tom Terwilliger
- Phenix: find_ncs.py(.bat) Tom Terwilliger
- Phenix GUI: Ralf W. Grosse-Kunstleve and Tom Terwilliger
- Web interface: Peter Zwart

Purpose

find_ncs finds potential operators NCS in (or the sites in a PDB file or (CC) a set of heavy-atom sites). If a PDB file is given, it can also find the sites of heavy atoms (Cl, Br, I, S, P, Se, Mn, Fe, Co, Ni, Cu, Zn) and use these to find NCS operators. If a model is given, it can also find the sites of solvent molecules (HOH) and use these to find NCS operators. If a set of heavy-atom sites is given, it can also find NCS operators from these heavy-atom sites.

How find_ncs works

The basic steps that find_ncs carries out are:

- Find the heavy-atom sites in the input pdb (used if the input file contains heavy-atoms or if the heavy-atom sites are specified in input) and find the solvent molecules (HOH) in the input pdb (used if the input file contains HOH or if the solvent sites are specified in input).
- Use either single sites (from pdb or PDBHEAD or find_hoh) or two sites (derived by search) to generate candidate NCS operators.
- Apply each candidate NCS operator to the sites and score the operator (derived by search or the input heavy-atom sites).
- Select the NCS operators and write out.

Output files from find_ncs

The output files that find_ncs produces are:

- NCS operators written in format for phenix.refine find_ncs.ncs
- NCS operators written in format for phenix.refine find_ncs.ncs_spec
- Model with solvent sites (if input was a model) find_ncs_output.pdb

What find_ncs needs

- find_ncs needs a file with map coefficients and optionally a second file containing NCS information.
- find_ncs needs a keyword file.

In order to run find_ncs you need to have a file with map coefficients for a map. If find_ncs does not choose the correct columns automatically, then you can specify them with a command like:

phenix find_ncs map_coeffs=myfile.mtz labels="fobs,phiobs"

phenix find_ncs map_coeffs=myfile.mtz

find_ncs has a number of options that you can have some sites and want to get operators, for example, you can tell find_ncs to ignore the map and:

find_ncs parameters.txtsites.txt

find_ncs parameters.txt sites.pdb

find_ncs parameters.txt sites.pdb ncs.ncs_spec

Format of NCS operators

The NCS operators look like this:

```
rotation
rot1(1)= 0.000  0.000  1.000
rot1(2)= 1.000  0.000  0.000
rot1(3)= 0.000  1.000  0.000
rotation
center(1)= 10.000  10.000  0.000
```

The rotation matrix is in orthogonal coordinates (Å) and the translation information, and center, pdb is (approximately) the center of the region where the operator applies.

The rotation in this .ncs_spec file is that the NCS operator is applied to copy (x,y,z) to copy (x,y,z) to copy (x,y,z) and the NCS operators can also specify frame (reference) and RMS and CC and operator (that RMS and CC are for).

Examples

Standard run of find_ncs

If you have just a map coefficients file you can say:

phenix find_ncs myfile.mtz

and find_ncs will look for NCS related domains in mtz map (two Fos, one Fos, density for more details on how it does this).

If you have a model and a map file, from the command line you can type:

phenix find_ncs pdb.pdb myfile.mtz

This will produce the following output:

```
Reading from file myfile.mtz
Using miller array: Fobs,PHIobs
Using miller array: FOM
Using miller array: HL,PHIHL
Using miller array: FOM
Using miller array: HL,PHIHL
Using miller array: FOM
Using miller array: HL,PHIHL
```

find_ncs_from_density

Finding NCS from density in a map with find_ncs_from_density

Author(s):

Tom Terwilliger, Pavel Afonine, Tom Terwilliger

Purpose:

find_ncs_from_density is a tool to identify NCS relationships directly from an electron density map specified with a CCP4 formatted map file. The NCS relationships are identified by finding the rotations and translations that the electron density, rotated and shifted, most resembles itself. The rotations and translations that are consistent with the electron density are then output.

Usage

How find_ncs_from_density works:

- The find_ncs_from_density algorithm first identifies potential locations of centers of pseudosymmetry in the density by searching for points that have high density and are surrounded by points that have high density.
- Then it uses only a subset of points in and around these potential centers of pseudosymmetry to identify the most likely rotations and translations that make the density most resemble itself. The rotations and translations that are consistent with the density are then output in a file in the format of the program LSQKAB. The rotations and translations are also output in a file in the format of the program MAPMAN.
- The rotations and translations are then used to find the corresponding asymmetric units and unique regions in the density, and output files are then written out.

Output files from find_ncs_from_density

find_ncs_from_density.ncs_spec: A file containing the ncs ncs_spec.phenix file in and the MAPMAN rotation/translation file ncs.ncs_spec.ncs_spec.rot. The ncs_spec.phenix file can be read and used directly by other phenix programs such as **phenix.ncs_search**. The ncs.ncs_spec.ncs_spec.rot file can be read and used in MAPMAN.

Example

Standard run of find_ncs_from_density:

Running find_ncs_from_density is easy. Enter the command line one-liner type:

```
phenix.find_ncs_from_density map_coeffs.mtz
```

Possible Problems

If your molecule is large, you may wish to increase the radius used for NCS identification (density, radius) and the number of points used in the rotation and translation calculation (nsigma, nsigma). Both are set by default to 1.0.

If your density has many NCS copies (for example, ten), you may wish to specify that ten ncs_copies.

If you want to have the program look much harder for NCS, try the keyword n_center_cubed (for some other keywords see below). This will cause the program to look at a number of points in the density that is equal to the number of centers cubed (instead of the usual one for each center).

Literature

- **Finding** and **crystallographic symmetry in density maps of macromolecular structures**, T.C. Terwilliger, Acta Cryst. D (2010) 66, 213-221.

List of all available keywords

```
find_ncs_from_density
  ncs_file
    ncs_file_name = None
    ncs_out = ncs.ncs_spec.phenix
                      Write ncs information to a file
                      If ncs_file_name is not specified, this is default. If
                      ncs_file_name is specified, ncs_file_name.ncs_spec.phenix
                      will be used instead. If ncs_file_name.ncs_spec.phenix
                      exists, it will be read and used.
    center_phi_in = None
                      Rotation about first axis of density to be used in
                      NCS search
    density_phi_in = None
                      Rotation about first axis of density to be used in
                      NCS search
    density_take = 1
                      Take every density_take point in density for
                      calculation of NCS. Default is 1 (all points). Use
                      larger values to speed up calculation. Values of
                      density_take of 2 or 3 are usually acceptable.
  output_files
    ncs_ccp4_map = ncs.ncs_search.ccp4
                      Output map file with ncs search of density
    ncs = None
                      Output ncs file
    ncs_out_file = ncs.ncs_spec.phenix
                      Output file with ncs in phenix ncs_spec format
    prune_ncs = True
                      If defined, ncs operations will be pruned to only file that shows
                      improvement in CC
    directory = .
                      Directory with results
    temp_dir = Temp_dir
                      Temporary work directory
    output_dir = .
                      Output directory where files will be written
  density_select
    density_radius = 10
                      Radius for density to be put into compute
    ncs_searchfrac = 0.5
                      Minimum searched density fraction, how many (default) radius
    ncs_searchradius = 10
                      Radius for density to be searched for rotations
    delta_phi = 5
                      Angular spacing of search
    n_center = None
                      Number of points to be used as centers
    nsigma_cutoff = None
                      Minimum number of NCS copies to look for
    nsigma_for_ncs = 1.0
                      Number of standard deviations in ncs_nsigma_for_ncs*n_ncs
    nsigma_for_ncs_in_fraction = None
                      Number of standard deviations in ncs_nsigma_for_ncs*n_ncs
    fraction_volume_for_ncs = 0.5
                      Minimum fraction of the asymmetric unit volume in NCS that against
                      which to compute
    ncs_in_density = True
                      Use the ncs in the ncs_spec.phenix file to find ncs in the
                      density. If ncs_in_density is not specified, the ncs in the
                      ncs_spec.phenix file will be used if it is present. If
                      ncs_in_density is set to False, the ncs in the
                      ncs_spec.phenix file will be ignored.
    ncs_search_centers_only = False
                      If set then use the density inside the unit cell. This causes the
                      program to look only at points in the density that are near
                      center mass
  find_points
    density_radius = 10
                      Radius for density to be put into compute
                      Radius for density to be put into compute
    n_center_find = None
                      Number of points to be used as centers for finding ncs
                      Number of points to be used as centers for finding ncs
    n_center_cubed = False
                      Number of points to be used as centers for finding ncs
                      Number of points to be used as centers for finding ncs
    n_ncs = 1.0
                      Number of ncs copies
                      Number of ncs copies
    nsigma_cutoff = 1.0
                      Minimum number of standard deviations in density to be
                      considered
    nsigma_for_ncs = 1.0
                      Minimum number of standard deviations in density to be
                      considered
    fraction_volume = 0.5
                      Minimum fraction of the asymmetric unit volume in NCS that
                      against which to compute
    n_ncs = 1.0
                      NCS coordinate grid nsamp in fractional square
  rotation_search
    n_rot = 1.0
                      Approximate total for the calculation of a search in the
                      rotation in a 3-D grid. The finer resolution, use a finer
                      grid
    output_rotation = False
                      output rotation
  general
    verbose = True
                      verbose output
    debug = False
                      Write out extra information
    total_memory = None
                      Total memory available
    max_cpu = None
                      Maximum number of cpu's to use
    n_center_cubed_keyword = False
                      Use the keyword n_center_cubed (see above) for number-cubed-item
                      keywords (for example, if n_center_cubed is set to 2 then the
                      program will use n_center = 8 if n_center is not specified).
                      nsigma_cutoff_keyword, nsigma_for_ncs_keyword, n_ncs_keyword,
                      n_center_find_keyword, n_center_keyword, n_center_find_keyword,
```

Finding and analyzing difference map peaks

Pelican-based Biocritical Movement for Integrated Bioinformatics

Contents:

- Overview
- Configuration
- Output
- List of all available keywords

Overview

pelican.find_peaks_feder is a utility for identifying peaks of interest in difference maps, typically at the end of a PHENIX refinement run. It can be used to automatically generate a list of potential ligand binding sites, water molecules and other features of interest, and keep a record of changes and recalculations over time. This information is presented in a tabular form, and can be exported to other programs for further analysis.

Configuration

The program requires only a PDB file and data (including R-free flags). The default options should be sufficient for most purposes, but can be changed for each large difference map (using mtzdump, mtz.dump, mtz.trim or fitpack) by creating the ccp4rc.cccf.

By default, peaks which overlap with the input atoms (within a cutoff distance) will not be included. If you want to find all peaks, which may include water molecules or ions, additional options are available by clicking the "Peak search" button.

If the input data are missing, the minimal input is simply the path to your model and data files (which tells the program to use default PHENIX output filenames). If you have changed the output prefix or have other non-default expected inputs, you can specify them in the available options, which are also listed below.

Output

A summary text will appear at the end of the run (not seen square scripts, since Linux files and buttons to view them are not implemented), and a table will be created (including a file "peaks.cccf.pkl" with details stored raw):

- 1D, 2D and 3D peaks (positive)
- 1D, 2D and 3D holes (negative)
- 3D solvent/ion peaks (positive)
- 3D solvent/ion holes (negative)
- 3D water/ion associated peaks

The program will also write the 2Fo-DFc, DFc-DFc, and processed 2F maskedmtz maps. Additional table and map files may be created if the corresponding options are enabled. Peak sites in PDB format, PyMOL or Coot scripts, or CSV files can be created.

List of all available keywords

```
model=model.pdb
data=data.cccf
include_peaks_over_cutoff = False
                            By default, the program will ignore peaks that are below a
                            cutoff distance from existing atoms. This option will
                            include all peaks, including those that are very close to
                            existing atoms. It should be used with caution, since
                            most of the peaks will be artifacts, but may be useful if
                            you are looking for ions or water molecules that are
                            already modeled in the PDB file. Any PHENIX output files
                            will be generated with the suffix "_all_peaks".
exclude_peaks_near_atoms = False
                            Alternate to the above option that applies only to
                            solvent/ion peaks.
use_phenix_if_possible = True
                            If True, use Phenix or ccp4/fitpack calculations if the
                            input data are in a format that can be read by Phenix.
                            Otherwise, use ccp4 programs.
write_pdb = True
write_map = True
write_peaks_table = peaks.txt
use_file = False            Use file in PHENIX GUI, not used on command line
peak
  resolution = 3.0
  peak_search_method = AUTOMATIC (CCP4) no gaussian neither otherwise
  exclude = False
  energy = None
  exclude_nearest_atoms = False
  skip_peak_generation = False
  keep_map = True           Write temp map out if True
  map_type
    fo_fc_map = None        Scope of fo_fc_map and fcalc_map
    fcalc_map = None
    fo_map = None
    high_resolution = None
    low_resolution = None
    map_cap = None
    sufficient_resolution = 3.0  Number beyond sufficient resolution, ignored when sufficient, and exceeding
                                 the data resolution
    remove_sites_near_ligands = False
    ligand_selection_criterion = None
    ligand_model_selection_criterion = None
    ligand_cutoff = 5.0         Cutoff distance for ligand
    force_generation_from_map_coeffs = False
    convert_to_non_generation_if_sufficient_peaks_found_from_other_methods = 0.5
    map_coeffs
      fo_minus_fc = None        Minimum number of reflections cutoff
      fo_fc_plus_fc = None      Minimum number of reflections cutoff
    peak_finding
      find_peaks_in_map = True  Turn on automatic peak search on the fo-fc difference map and/or on exactly
                                the input coordinates
      keep = None
      peak_cutoff = None        Specify if fo-fc map was built by phenix or also generated
      find_filtered_peaks = None
                                Peaks which do exactly correspond exactly to the input atoms
                                (within some small cutoff) are ignored
      specify_fo_fc_peak_cutoff = False
                                Use a different cutoff for difference peaks and holes
      exclude_nearest_atoms = False
      peak_grid_factor = 1.0    If > 1.0, increase sampling density around the PDB Pseudogeneric Coordinate on
                                the fo-fc difference map
      peak_cutoff = 3.0         Sigmoid Minimum Peak cut off for detection of ligand sites
      hole
        resolution = None
        min_frac = None
        hole_cutoff = None      Default 0.5(fo)/ sigma (FOM)
        use_cutoff_sigmoid = True
        use_detected_centers = True
        use_detected_centers_if_no_hole_found = True
      use_peaks_in_solvent_mask = True
                                Use the found peaks in the solvent mask and recalculate the solvent mask
                                and maskedmtz
      use_peaks_in_solvent_mask_and_recalculate_maskedmtz = True
                                Use the found peaks in the solvent mask and recalculate the solvent mask
                                and maskedmtz
      find_peaks_in_solvent_mask = False
                                Find peaks in the solvent mask
      use_peaks_in_solvent_mask_for_ccp4 = False
                                Use the found peaks in the solvent mask for ccp4 calculations
      use_peaks_in_solvent_mask_for_phenix = False
                                Use the found peaks in the solvent mask for phenix calculations
      use_peaks_in_solvent_mask_for_both = False
                                Use the found peaks in the solvent mask for both ccp4 and phenix calculations
      use_peaks_in_solvent_mask_for_both_and_recalculate_maskedmtz = False
                                Use the found peaks in the solvent mask for both ccp4 and phenix calculations
                                and recalculate maskedmtz
      find_peaks_in_solvent_mask_and_use_for_other_peaks = False
                                Find peaks in the solvent mask and use them for other peaks
      find_peaks_in_solvent_mask_and_use_for_other_peaks_and_recalculate_maskedmtz = False
                                Find peaks in the solvent mask and use them for other peaks and recalculate
                                maskedmtz
      use_peaks_in_solvent_mask_and_recalculate_maskedmtz = False
                                Use the found peaks in the solvent mask and recalculate maskedmtz
      use_peaks_in_solvent_mask_and_recalculate_maskedmtz_and_use_for_other_peaks = False
                                Use the found peaks in the solvent mask and recalculate maskedmtz and use
                                them for other peaks
      use_peaks_in_solvent_mask_and_recalculate_maskedmtz_and_use_for_other_peaks_and_recalculate_maskedmtz
                                = False
                                Use the found peaks in the solvent mask and recalculate maskedmtz and use
                                them for other peaks and recalculate maskedmtz
      use_peaks_in_solvent_mask_and_recalculate_maskedmtz_and_use_for_other_peaks_and_recalculate_maskedmtz_and_use_for_other_peaks
                                = False
                                Use the found peaks in the solvent mask and recalculate maskedmtz and use
                                them for other peaks and recalculate maskedmtz and use them for other peaks
      use_peaks_in_solvent_mask_and_recalculate_maskedmtz_and_use_for_other_peaks_and_recalculate_maskedmtz_and_use_for_other_peaks_and_recalculate_maskedmtz
                                = False
                                Use the found peaks in the solvent mask and recalculate maskedmtz and use
                                them for other peaks and recalculate maskedmtz and use them for other peaks
                                and recalculate maskedmtz
      use_peaks_in_solvent_mask_and_recalculate_maskedmtz_and_use_for_other_peaks_and_recalculate_maskedmtz_and_use_for_other_peaks_and_recalculate_maskedmtz_and_use_for_other_peaks
                                = False
                                Use the found peaks in the solvent mask and recalculate maskedmtz and use
                                them for other peaks and recalculate maskedmtz and use them for other peaks
                                and recalculate maskedmtz and use them for other peaks
    peak
      resolution = None
      min_frac = None
      peak_cutoff = None        Default 0.5(fo)/ sigma (FOM)
      use_cutoff_sigmoid = True
      use_detected_centers = True
      use_detected_centers_if_no_hole_found = True
    n_peaks = 10
    n_holes = 10
  pdb
    file_name = None          Model filter name (PDB)
  mtzdump
    file_name = None          Mtzdump filter name (.log)
  map
    map_file_name = None      A file-formatted map
    map_type = None           Map type (ccp4, phenix, or
    map_coefficients_file_name = None
                              Map coefficients file
    map_coefficients_labels = None
                              Labels for map coefficients in MTZ file
find_peaks
  use_phenix_if_possible_mtz = True
                              Default is ccp4 unless map, map in absolute scale is used otherwise.
  write_mtz = True            Write map to map coefficients
  mtz_prefix = None
  mtz_suffix = None
  map_mtz_to_make
    map_name_prefix_and_suffix = None
    map_name_prefix_only = None
    map_name_suffix_only = None
    map_name_prefix_and_suffix_and_prefix = None
    map_name_suffix = None
    map_name = None
  output
    output_to_log = True
    output_to_stdout = True
    output_to_file = True
    general_precision_only = False
    write_to_log_file = True
    write_to_stdout = True
    write_to_file = True
```

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

Finding a program or test using find_program

Author(s)

- The program: Ralf Grosse-Kunstleve

Purpose

The module find_program will show all the programs that match supplied text (either in program name or in program description). The locations of the programs (which lie in the field or command line tree) are shown.

Optionally, the module will show the source code of the matching program or search in the source of the code based on the name of a function that is called by the matching program.

Lastly, find_program can find all the Python programs that have changed since last checkpoint in programs in the Python tree, and can also keep a checkpoint file for such changes.

Usage

How find_program works:

Searches for programs:

find_program uses the list of programs and short descriptions in the file
/Users/nigel/cctbx/modules/phenix/phenix/command_line/phenix_dist.py. The program names, keywords, or complete program names are separated from WORD/KEYWORD/PROGRAMNAME/DESCRIPTIONS/PROGRAMNAME_LONG_DESCRIPTION by the character "|" in the file phenix_dist.py.

find_program then makes a list of all programs, descriptions, and locations.
It then finds the matching programs and prints out the information.

Searches for regression tests:

find_program can also look for and display regression tests. It displays find_and_include_info.py of
/Users/nigel/cctbx/modules/phenix/phenix/regression/find_and_include_info.py
which contains programs and their associated tests. This database is built by find_program and can be specified either by special arguments to find_program or automatically by including the text "find" in the keywords. Note: the keywords are separated by the character "|" in the file phenix_dist.py, as described above.

The search for regression tests by module is a way to find a test that will run a module that you are interested in.

Search for regression tests affecting all changed programs:

find_program can find all the Python programs that have changed since the last check in (or since a given date). It can also find the regression tests that are associated with these programs. It can also run the regression tests in this

find_program can also find all the tests that could possibly fail due to any changed Python modules. Note that this search will not find tests that may be affected, but it does find tests that is possible to fail when using the changed modules. It can also find tests that do not have such dependencies.

Running regression tests

The existing regression tests are stored in the module tests in directory /Users/nigel/cctbx/modules/phenix/phenix/regression/tests/. This directory holds find_program if you use the -p or -ptest options.

Standard use of find_program:

You can use find_program to find a program like this:

phenix.find_program keywords

You can also use it to find find a keyword that that overlaps a module with the exact extensions to it (phenix.find and also find some regular expressions.

phenix.find_program -p phenix.find -p phenix.find_program -p phenix.find_program -p phenix.find_program

Setting up the database for find_program:

You can update the database for find_program by running the test

phenix.regression.find_and_include_info tests/dist

in an empty directory. This will take a while (perhaps an hour or so with rpms-lib) and produce a file called find_and_include_info.pkl.

You can copy this file to offline location or

/PHENIX/modules/phenix/phenix/regression/find_and_include_info.pkl

and then find_program will use this new version. You can also specify where this pkl file is located with the command line

phenix.find_program -d find_and_include_info.pkl

Possible Problems

Specific limitations and problems:

The Python version of phenix.find_program has problems do not find C++ code that is affected by a test that changes Python.

Literature

Additional information

List of all available keywords

```
phenix.dist                     find_program keywords
phenix.find_program             find keywords here to cover all changed Python files in phenix
phenix.find_program -p phenix.find -p phenix.find_program -p phenix.find_program -p phenix.find_program
                                  -d find_and_include_info.pkl
                                  -ptest -d find_and_include_info.pkl -v -v -v
```

fit_loops

Phenix

Python-based Hierarchical Environment for Integrated Crystallography

Fitting loops to fit in gaps in models with fit_loops

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Author(s)

Tom Terwilliger

Purpose

fit_loops is a tool for building a loop into density to connect existing chain ends. You supply a model with a gap, density, and information about the connection between the ends of the gap, and fit_loops will try to build a loop to fill the gap. If the loop will attempt to build the loop and check to see if it fits well into the density. If it does, it will write out the model with the loop added. If it does not, it will write out the model with the loop added and a warning.

You can also define a loop library to be used for the loop. By default fit_loops uses beams-shaped alpha-helices to try to build loops. If you have a library of loop fragments that are appropriate for your data and structure, fit_loops will try to find the best one to use. You can also specify a particular loop from the library to be used, or specify that fit_loops should not use any loops from your loop library.

If you have a gap in your complex model-building process, then you will want to try phenix.autobuild.

To show you how to use fit_loops we provide the PHENIX 2013

Usage

How fit_loops works:

fit_loops calculates a new model on the original map coefficients. Then it tries to extend the ends of the supplied model into the gap, using the new model as a template.

Output files from fit_loops:

fit_loops.pdb, fit_loops.mtz: The output from fit_loops is a new PDB file containing your input model with the loop added, and the corresponding map coefficients.

Examples

Standard run of fit_loops:

A typical command line input would be:

```
phenix.fit_loops pdb_in=input.pdb mtz_in=input.mtz
  mtz_out=fit_loops.mtz pdb_out=fit_loops.pdb
```

This will read the input model from input.pdb and the corresponding F,PHI map coefficients from input.mtz and will write out the new model with the loop added to fit_loops.pdb and the corresponding map coefficients to fit_loops.mtz. If the loop does not fit well into the density, a warning will be written out to the screen.

Specifying column names

If you want to specify which column in the input mtz file you will need to tell fit_loops what F and PHI to use:

```
phenix.fit_loops pdb_in=input.pdb mtz_in=input.mtz
  mtz_out=fit_loops.mtz pdb_out=fit_loops.pdb
  mtz_in.labels="F,PHI"
```

Fitting a loop with poor density

If you want to try and fit a loop with poor density, you might want to lower the threshold for the correlation of the loop with the density and increase the number of trials:

```
phenix.fit_loops pdb_in=input.pdb mtz_in=input.mtz
  mtz_out=fit_loops.mtz pdb_out=fit_loops.pdb
  loop_cc_cutoff=0.3 loop_ntrial=100
```

Using a loop library to correct all segments

To use the loop library in PHENIX, use the keyword loop_lib:

```
phenix.fit_loops pdb_in=input.pdb mtz_in=input.mtz
  mtz_out=fit_loops.mtz pdb_out=fit_loops.pdb
  loop_lib=yes
```

This will try to fit each gap in the model using the loop library, and will replace any segments that do not fit well with the loop from the library.

Using a loop library to correct all segments

To use the loop library in PHENIX and try to correct any part of segments that have an geometrical relationship, use the keyword loop_lib_all:

```
phenix.fit_loops pdb_in=input.pdb mtz_in=input.mtz
  mtz_out=fit_loops.mtz pdb_out=fit_loops.pdb
  loop_lib_all=yes
```

This will try to fit each gap in the model using the loop library, and will replace any segments that do not fit well with the loop from the library. Note that this is more liberal approach, normally chosen only if you have a good loop library and want to use it as much as possible.

Specifying a gap to fill in

To specify a particular gap for loop fitting, you can use:

```
phenix.fit_loops pdb_in=input.pdb mtz_in=input.mtz
  mtz_out=fit_loops.mtz pdb_out=fit_loops.pdb
  gap_to_fill="A:10-A:15"
```

Note that because number the start and end are the first and last of the gap, not the residues flanking the gap. Also note that the chain ID is required. If you want to specify a gap in a multi-chain model, you can specify the gap in the form of chain1:start-chain2:end, specifying residues chain1:start and chain2:end as the first and last residues in the gap.

Possible Problems

One of the most common problems is that the replacing loop lacks backbone and other or gaps are interpolated poorly. Based on the input model, fit_loops will try to extend the ends of the gap and build a loop that connects the ends. If the ends are not in the correct orientation, fit_loops will fail. Also, if the loop does not fit well into the density, fit_loops will warn you that the loop does not fit well.

If the loop does not fit well into the density, fit_loops will try to find a better loop. If you want to force fit_loops to use a particular loop, you can specify the loop to be used with loop_id=.

You can also recommend that fit_loops try the specified loop, even if it looks poor, with the flag force_loop=yes.

Note that phenix.fit_loops has a number of options, which can be listed by typing phenix.fit_loops -h.

Specific Applications and problems:

Literature

Additional information

List of all available keywords

```
model_file=None
  pdb_in = None                 PDB file with gap to fill.
  mtz_in = None                 Input MTZ file with coefficients for a map
  pdb_out = None                PDB file with loop added.
  mtz_out=fit_loops.mtz         Output MTZ file with map coefficients for the loop-fitted
                                model. If the input model is a multi-chain model, the
                                output model will be written out in the form of a single
                                chain with residues numbered from 1 to the number of
                                residues in the input model. If the input model is a
                                multi-chain model, the output map coefficients will be
                                calculated on the PDB file that has the symmetry. Because the output
                                model may be different than the input model, the output map
                                coefficients may not be appropriate for the input model.
  labels = "F"                  Input map coefficients to use (F,PHI)
  mtz_out_labels=None           Output labels for map coefficients
  mtz_out_type=None             Output file type (map, map_coef or mtz_phase)
  loop_lib = None               File containing loop library
  loop_id = None                Use only loop with this number (begins at zero)
  loop_cc_cutoff = 0.5          Minimum correlation of loop with density to accept
  loop_ntrial = 10              Number of trials to try for each loop
  loop_rms = 0.5                Rms deviation of loop from ideal geometry
  loop_ntrial_rms = 100         Number of trials to try for each loop if geometry
                                is not good
  force_loop = False            Force use of loop even if it does not fit well
  gap_to_fill=None              Gap to fill in (chain1:start-chain2:end, where
                                chain1:start and chain2:end are the last and first
                                residues in the gap. Chain IDs are required. If more
                                than one gap is in the model, this will be used to
                                select the gap to be filled. If not specified, the
                                first gap will be filled.)
  loop_lib_all = False          Use loop library to correct all segments of loop
                                that are in a geometrical relationship with a loop
                                in the library (rms deviation of bond lengths and
                                bond angles of 0.5 or less)
  loop_lib = False              Use loop library to correct any segments that do not
                                fit well (rms deviation of bond lengths and bond
                                angles of 0.5 or more)
  start = None                  Start of loop to be fitted (chain1:start-chain2:end
                                where chain1:start and chain2:end are the last and
                                first residues in the gap. Chain IDs are required.
                                If more than one gap is in the model, this is used
                                to select the gap to be filled. If not specified,
                                the first gap will be filled.)
  end = None                    End of loop to be fitted (chain1:start-chain2:end
                                where chain1:start and chain2:end are the last and
                                first residues in the gap. Chain IDs are required.
                                If more than one gap is in the model, this is used
                                to select the gap to be filled. If not specified,
                                the first gap will be filled.)
  chain_id_in_model=None        Chain ID in model to be used for fitting (optional
  remove_loop = True            Remove existing loop in model (if present)
  skip_fit = True               Skip fitting loop (just write out model with
                                existing loop and map coefficients)
  write_log = True              Write log file (fit_loops.log)
  verbose = False               Verbose output
  n_trial = 10                  Number of trials to try for each loop
  n_cycle = 3                   Number of cycles of refinement
  n_cycle_rms = 3               Number of cycles of refinement if rms deviation
                                of loop is too high
  n_cycle_cc = 3                Number of cycles of refinement if correlation of
                                loop with density is too low
  rms_max = 0.5                 Maximum rms deviation of bond lengths and bond
                                angles for loop to be considered good
  cc_min = 0.5                  Minimum correlation of loop with density to be
                                considered good
  cc_min_rms = 0.3              Minimum correlation of loop with density to be
                                considered good if rms deviation of bond lengths
                                and bond angles is 0.5 or less
  cc_mask = 0.5                 Radius around atoms to mask for calculating
                                correlation of loop with density
  cc_mask_rms = 0.3             Radius around atoms to mask for calculating
                                correlation of loop with density if rms deviation
                                of bond lengths and bond angles is 0.5 or less
  cc_ncyclic = 3                Number of cycles of smoothing for calculating
                                correlation of loop with density
  cc_ncyclic_rms = 3            Number of cycles of smoothing for calculating
                                correlation of loop with density if rms deviation
                                of bond lengths and bond angles is 0.5 or less
  n_ca_start = 3                Number of CA atoms at start of loop to fit
  n_ca_end = 3                  Number of CA atoms at end of loop to fit
  max_density_of_points = None  Maximum density of points to consider in analysis
                                of loop
  min_density_of_points = None  Minimum density of points to consider in analysis
                                of loop
  n_points = 100                Number of points to use in analysis of density
  n_points_rms = 50             Number of points to use in analysis of density if
                                rms deviation of bond lengths and bond angles is
                                0.5 or less
  weight = 1                    Weight for bond and bond angle terms in target
                                function
  min_dist = 2.5                Minimum distance for a clashing atom
  max_dist = 4.0                Maximum distance for a clashing atom
  max_n_clash = None            Maximum number of clashing atoms
  max_n_clash_rms = None        Maximum number of clashing atoms if rms deviation
                                of bond lengths and bond angles is 0.5 or less
  n_clash_for = None            Number of clashing atoms to use in clash score
                                calculation
  n_clash_for_rms = None        Number of clashing atoms to use in clash score
                                calculation if rms deviation of bond lengths and
                                bond angles is 0.5 or less
  n_cycle_clash = 3             Number of cycles of refinement if clashes are
                                present
  n_cycle_clash_rms = 3         Number of cycles of refinement if clashes are
                                present and rms deviation of bond lengths and bond
                                angles is 0.5 or less
  n_cycle_fit = None            Number of cycles of refinement to fit loop
  n_cycle_fit_rms = None        Number of cycles of refinement to fit loop if rms
                                deviation of bond lengths and bond angles is 0.5
                                or less
  n_cycle_fit_cc = None         Number of cycles of refinement to fit loop if
                                correlation of loop with density is 0.5 or less
  n_cycle_fit_cc_rms = None     Number of cycles of refinement to fit loop if
                                correlation of loop with density is 0.5 or less
                                and rms deviation of bond lengths and bond angles
                                is 0.5 or less
  n_cycle_fit_clash = None      Number of cycles of refinement to fit loop if
                                clashes are present
  n_cycle_fit_clash_rms = None  Number of cycles of refinement to fit loop if
                                clashes are present and rms deviation of bond
                                lengths and bond angles is 0.5 or less
  n_cycle_final = None          Number of cycles of refinement to fit final loop
  n_cycle_final_rms = None      Number of cycles of refinement to fit final loop
                                if rms deviation of bond lengths and bond angles
                                is 0.5 or less
  n_cycle_final_cc = None       Number of cycles of refinement to fit final loop
                                if correlation of loop with density is 0.5 or less
  n_cycle_final_cc_rms = None   Number of cycles of refinement to fit final loop
                                if correlation of loop with density is 0.5 or less
                                and rms deviation of bond lengths and bond angles
                                is 0.5 or less
  n_cycle_final_clash = None    Number of cycles of refinement to fit final loop
                                if clashes are present
  n_cycle_final_clash_rms = None Number of cycles of refinement to fit final loop
                                if clashes are present and rms deviation of bond
                                lengths and bond angles is 0.5 or less
  force_loop = False            Force use of loop even if it does not fit well
  loop_id = None                Use only loop with this number (begins at zero)
```

fix_insertions_deletions

Phonix Phonetic Sound Processor Phonetics for Advanced Bioinformatics

Fixing regular errors in a model with fix_insertions_deletions

Author(s)

Dr. Stefan Seemann, Dr. Kai Tetzlaff

Purpose

The module fix_insertions_deletions is a tool for fixing regular errors in a model by comparing the density at each state additions to a separate file.

Usage

This module will amend the functionality of the_insertion_deletions by running the Phonix tools, fix_model tool in the Phonix GUI. However you can run it directly as well (Phonix is not GUI for fix_insertions_deletions).

How fix_insertions_deletions works:

The module fix_insertions_deletions fixes regular errors in a model by comparing the density at each state insertion or deletion to a separate file which includes corresponding to each segment in the model.

These state insert probabilities are used to generate a new hidden sequence for the model and map. This map is then used to generate a new model. Since the new model is based on the old model, the new model inherits it. Hence, to be correct, and what changes in regards are needed to fix it.

Each state in hidden shift is marked in order as a target for state insertion. Deletions indicating the specified state in the hidden shift are marked as a source. Insertions are marked as a target and deletions as a source.

Additional rebinding of the state fitting regions is also carried out.

Using fix_insertions_deletions:

fix_insertions_deletions is a command line tool, runs automatically as part of Phonix, and, both however you can run it yourself by using the arguments:

Input map file: The map file should cover the model you supply.

Input Sequence: Supply the sequence of your map (usually the sequence derived by your half-pressed Fourier shell correlation.

Model: Supply a model that you want to fix. Only the chain chain will matter.

Sequence: Supply a sequence file that covers at least part of the model that is supplied

Examples

Standard run of fix_insertions_deletions:

./fix_insertions_deletions -m model.pdb -s seq.fasta -i map.ccp4 -o out.pdb -d dens.dat

Possible Problems

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
[ALIGN]
  align_file = Text
  align_type = Text
  align_mode = Text
  align_fill = Text
  alignment_global_file = Text
[ANGLE_TEAM]
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[DEP]
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  interface_cutoff_file_type = Text
  interface_cutoff_file_type_prefix = Text
  interface_cutoff_chain_file = Text
  interface_cutoff_chain_file_prefix = Text
  interface_cutoff_chain_file_type = Text
  interface_cutoff_chain_file_type_prefix = Text
  interface_cutoff_chain_selection_file = Text
  interface_cutoff_chain_selection_file_prefix = Text
  interface_cutoff_chain_selection_file_type = Text
  interface_cutoff_chain_selection_file_type_prefix = Text
  interface_cutoff_residue_selection_file = Text
  interface_cutoff_residue_selection_file_prefix = Text
  interface_cutoff_residue_selection_file_type = Text
  interface_cutoff_residue_selection_file_type_prefix = Text
  interface_cutoff_atom_selection_file = Text
  interface_cutoff_atom_selection_file_prefix = Text
  interface_cutoff_atom_selection_file_type = Text
  interface_cutoff_atom_selection_file_type_prefix = Text
[INTERFACE_DIST]
  interface_dist = Text
  interface_dist_prefix = Text
  interface_dist_type = Text
  interface_dist_type_prefix = Text
  interface_dist_chain = Text
  interface_dist_chain_prefix = Text
```

PhenoIS *Phenotypic Hierarchical Measurement for Integrated Multiparametric Screening*

Find matching fragments in the PDB (fragment_search)

Author(s)

- fragment_search: Tom Terwilliger

Purpose

Find a fragment from the PDB that is similar to a segment in a supplied model.

Fragment_search finds a short segment of model similar to one that interest a segment in a preliminary model by replacing it with a similar fragment from a deposited structure.

Note that fragments from the PDB may not actually have good geometry because it is incorrect (distorted) to fit the PDB data.

Fragment_search differs from cryoem_refit_fragments_from_pdb in that fragment_search is looking for a single fragment that matches a segment of a model, while cryoem_refit_fragments_from_pdb is looking for fragments that are a string of consecutive residues and a model that is a set of fragments.

Usage

Fragment_search can find a fragment in the PDB similar to a supplied fragment (protein chains only)

Fragment_search finds the maximum number of matches/distances in the replacement fragment and similar to match the fragment.

You can also specify keywords to exclude or include specific PDB entries or exclude all PDB entries with sequences similar to a particular PDB entry.

You can choose to create a replacement fragment (or just a distorted part of your model) by supplying a selection string. Default is no replacement.

How fragment_search works:

Fragment_search is done using a quick Cbeta-only set of chains from the PDB filtered at 90% sequence identity. Fragments are found by superimposing the Cbeta atoms of the fragment on the Cbeta atoms of the chains and accepting up to 100 fragments with good geometry. The main chain coordinates of these structures are supplied to the main fragment_search.

Potential matching fragments are found by comparing end-to-end distances for the length with all fragments of the same length in the PDB. Fragments are then superimposed on the supplied fragment and the RMSD is calculated by comparing of distances from end to middle (internal distances) of the target fragment. Further tests are then carried out on the target fragment, including to select the target fragment, and the fragment is then superimposed on the supplied fragment.

Matching residues are then found by finding the fragment in sliding mode and an alternate sliding mode by using the fragment as a target for the fragment in the PDB and finding the residues that are within 1.5A of one of the target fragment.

Residues in the matching fragment are assigned to the matching fragment in order to make sense to the target fragment. For this purpose residues of variable or of a very similar type are assigned to the matching fragment. Residues are then assigned to a particular residue (alanine, Cbeta length), and replacing the identified residues and the atoms in the matching fragment.

Examples

Standard run of fragment_search:

- phenix.fragment_search model.pdb fragment.pdb output.pdb
- phenix.fragment_search model.pdb fragment.pdb output.pdb keep_type=T

The old file fragments in the PDB similar to residues 1-20 of model.pdb:

Possible Problems

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
  ON_ERROR = None
    keep_type = False
      Keep the type of the matching residues
    ATOMTYPE = None
      Use this atomtype
    replacement_mode_prefix = None
      Replace first and replacement model with these prefix

  fragment_search
    model = None
      Model
    fragment = None
      Fragment
    max_count = 1
      Maximum number of fragments to find
    max_gap = 10
      Maximum gap in chain
    min_fragment_matching_by_distances = 0.8
      Minimum fraction of distances to be matching
    max_rms = 1.5
      Maximum rms for superimposed fragments
    min_rms = 0.5
      Minimum rms for superimposed fragments
    max_distance = 3
      Maximum distance to search
    pdb_include_text = None
      Only use PDB if its pdb ID and chain id is include (OR) in this list
    pdb_exclude_text = None
      Exclude PDB if its pdb ID and chain id is include (OR) in this list
    pdb_same_as_fragment_pdb_id_only = False
      Only use PDB entry with same pdb id as fragment
    pdb_same_as_fragment_pdb_id_and_chain_id = False
      Only use PDB entry with same pdb id and chain id as fragment
    keep_all_chains = False
      Keep all chains
    replace_with_identical_fragment = False
      Replace with identical fragment if found
    replace_with_similar_fragment = False
      Replace with similar fragment if found
    replacement_fragment = None
      Replacement fragment
    replacement_fragment_pdb = None
      Replacement fragment pdb
    replacement_fragment_chain = None
      Replacement fragment chain
    replacement_fragment_selection = None
      Replacement fragment selection
    replacement_fragment_id = None
      Replacement fragment id
    replacement_fragment_rms = None
      Replacement fragment rms
    replacement_fragment_matching_by_distances = None
      Replacement fragment matching by distances
    replacement_fragment_rms_to_target = None
      Replacement fragment rms to target
    replacement_fragment_matching_by_distances_to_target = None
      Replacement fragment matching by distances to target
    max_fragments = 100
      Maximum number of fragments to search
    min_fragments = 1
      Minimum number of fragments to search
    max_distance_for_fragment_selection = 3.0
      Maximum distance for selection of fragment
    min_distance_for_fragment_selection = 0.5
      Minimum distance for selection of fragment
    max_fragment_matching_by_distances = 0.8
      Maximum fraction of distances to be matching
    min_fragment_matching_by_distances = 0.5
      Minimum fraction of distances to be matching
    max_fragment_rms = 1.5
      Maximum rms for superimposed fragments
    min_fragment_rms = 0.5
      Minimum rms for superimposed fragments
    max_fragment_distance = 3
      Maximum distance to search
    min_fragment_distance = 0.5
      Minimum distance to search
    fragment_selection = None
      Fragment selection
    fragment_id = None
      Fragment id
    fragment_rms = None
      Fragment rms
    fragment_matching_by_distances = None
      Fragment matching by distances
    fragment_rms_to_target = None
      Fragment rms to target
    fragment_matching_by_distances_to_target = None
      Fragment matching by distances to target
    replacement_mode = False
      Replacement mode
    replacement_selection = None
      Replacement selection
    replacement_id = None
      Replacement id
    replacement_rms = None
      Replacement rms
    replacement_matching_by_distances = None
      Replacement matching by distances
    replacement_rms_to_target = None
      Replacement rms to target
    replacement_matching_by_distances_to_target = None
      Replacement matching by distances to target
    replacement_type = None
      Replacement type
    replacement_keep_type = None
      Replacement keep type
    replacement_keep_atomtype = None
      Replacement keep atomtype
    replacement_keep_chain = None
      Replacement keep chain
    replacement_keep_selection = None
      Replacement keep selection
    replacement_keep_id = None
      Replacement keep id
    replacement_keep_rms = None
      Replacement keep rms
    replacement_keep_matching_by_distances = None
      Replacement keep matching by distances
    replacement_keep_rms_to_target = None
      Replacement keep rms to target
    replacement_keep_matching_by_distances_to_target = None
      Replacement keep matching by distances to target
```

geometry_minimization

phenix.geometry_minimization: regularize model geometry

Description

This program applies chemical geometry restraints to standard geometry restraints.

In addition it can use extra restraints such as:

- secondary structure
- reference coordinates
- reference torsion angles
- cross-validation restraints
- Ramachandran and rotamer chiralty restraints
- NCS restraints and rotamer restraints

Command line phenix.geometry_minimization

```
phenix.geometry_minimization model.pdb
```

Alias

phenix.real_space_refine is available

List of all available keywords

```
output = None
output_dir = None
file_name = None
overwrite = False
nproc = None
nproc_gui = None
output_file_name_prefix = None
directory = None
file_name = None
log_level_verbosity = True
write_log_file = True
output_log = None
output_cif = None
output_mtz = None
output_pdb = None
output_pdb_precision = None
write_pdb_header_records = True
write_pdb_remark_1_record = True
precision = 1
write_cif_header = True
write_cif_data = True
write_cif_precision = None
write_cif_mtz_data = True
write_cif_pdb_data = True
write_cif_pdb_precision = None
write_cif_pdb_header_records = True
write_cif_pdb_remark_1_record = True
write_cif_pdb_remark_1_precision = None
write_mtz_data = True
write_mtz_pdb_data = True
write_mtz_pdb_header_records = True
write_mtz_pdb_remark_1_record = True
write_mtz_pdb_remark_1_precision = None
write_pdb_header_records = True
write_pdb_remark_1_record = True
write_pdb_remark_1_precision = None
write_log_header_and_footer = True
write_log_header_and_footer_only = False
write_log_header_and_footer_only_if_interesting = False
write_log_level = 1
write_log_interesting_only = False
suppress_output = False
write_output_files = True
dry_run = False
output_geometry_restraints = False
output_geometry_restraints_file = None
suppress_logging = False
write_geometry_restraints_files = True
write_geometry_restraints_files_name = None
write_geometry_restraints_files_append = False
verbose = True
  log = Information Dependent Library (IDL) for geometry restraints
  title = Input PDB file
  description = Input PDB file
  type = str
  multi = False
  input_by_user = False
  gui = False
  output_text = None
  wizard = False
  optional = False
  style = file_name
  add_extension = None
  add_to_output = False
  default = None
  type = str
  multi = False
  input_by_user = False
  gui = False
  output_text = None
  wizard = False
  optional = True
```

```
include_in_accounts_listing
  enabled_by_default: true
  enforced: false
  order: 1
  display_name: "Accounts listing"
exclude_from_accounts_listing
  enforced: false
  order: 2
  display_name: "Exclude from accounts listing"

apply_city_state_specification
  enabled_by_default: false
  enforced: false
  order: 1
  display_name: "Apply city state specification"
apply_city_state_exceptions
  enabled_by_default: false
  enforced: false
  order: 2
  display_name: "Apply city state exceptions"
apply_city_state_specification_for_exceptions
  enabled_by_default: false
  enforced: false
  order: 3
  display_name: "Apply city state specification for exceptions"
exclude_from
  [redacted]
  [redacted]
  [redacted]
```

#phenix-keywords #Reflections #Phasing #Crystallography

Correlation of two maps (deprecated, use MapCorrelations)

Author(s)

- Pavel V. Afonine, Tom Terwilliger

Purpose

get_cc_mtz_mtz is a command line tool for calculating the angle or a map so that the map superimposes on another map, and for calculating the correlation of the two maps. The maps are obtained from map coefficients supplied in the input mtz files.

Usage

How get_cc_mtz_mtz works:

get_cc_mtz_mtz calculates map based on the supplied mtz files. Even uses NCS(NCS) to find the origin shift. Compatible with space group symmetry that maximizes the correlation of the two maps. The shift is applied to the second map to maximize the correlation with the first map.

Several parameters can be set to the user to define how the correlations are calculated. By default, maps are calculated on the unit cell. Alternatively, calculation on the bigger box (selected from 2 mtz) is also possible.

If you specify

```
map_cutoff,sphere_around_at_xyz_cutoff=0.5
```

Then the map calculated using your second mtz file will only include reflections that were present in your first mtz file. This will reduce the effects of missing reflections in the correlation.

If you specify

```
sphere=10
```

Then the map calculated using your second mtz file will only include reflections that were present in your first mtz file and lie within 10 Å of a sphere centered on the correlation.

If you specify

```
keep_together
```

then get_cc_mtz_mtz uses analysis from the first input mtz file and phases and figure of merit from both mtz files to calculate the correlation. This will reduce the effects of differences in amplitudes on the correlation, and focusing on differences in phases and figures of merit.

Output files from get_cc_mtz_mtz

- Output: Correlation between two maps calculated.

Examples

Standard run of get_cc_mtz_mtz:

Running the get_cc_mtz_mtz is easy. Type the command line you can type:

```
phenix.get_cc_mtz_mtz map_coeffs_1.mtz map_coeffs_2.mtz
```

If you do not specify any parameters, it will ask for the name of the map file, you will need to call get_cc_mtz_mtz what map coefficients you want to use for the map calculation:

```
phenix.get_cc_mtz_mtz map_coeffs_1.mtz map_coeffs_2.mtz
map_coeffs_1.mtz,map_coeffs_2.mtz,map_coeffs_2.mtz,map_coeffs_2.mtz
```

Possible Problems

Specific limitations and problems:

- Absence of phases get_cc_mtz_mtz can fail if asked a different set of defaults, with the values,

```
keep_together=1
map_cutoff,sphere_around_at_xyz_cutoff=0.5
```

These defaults were changed after version 1.10-beta-2 in order to make the results independent of the order of the mtz files and to allow the default to be set for calculation of large reflections.

List of all available keywords

```
get_cc_mtz_mtz
  .type = command
  .help = Help
  .short_caption = Help
  .enum = Help
  .expert_level = 0

  map_1 = None
  .type = path
  .multi = False
  .output_to_cwd = False
  .input_type = map_coeffs
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  map_2 = None
  .type = path
  .multi = False
  .output_to_cwd = False
  .input_type = map_coeffs
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  map_cutoff = None
  .type = float
  .multi = False
  .value_min = 0.0
  .value_max = 1.0
  .allow_none = True
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  sphere = None
  .type = float
  .multi = False
  .value_min = 0.0
  .value_max = None
  .allow_none = True
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  sphere_around_at_xyz_cutoff = None
  .type = float
  .multi = False
  .value_min = 0.0
  .value_max = 1.0
  .allow_none = True
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  keep_together = None
  .type = bool
  .multi = False
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  shift_cutoff = None
  .type = float
  .multi = False
  .value_min = 0.0
  .value_max = None
  .allow_none = True
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  use_cell = None
  .type = bool
  .multi = False
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  use_ncs = None
  .type = bool
  .multi = False
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  output_cmdline_full = None
  .type = bool
  .multi = False
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  .help = Write full command line to output
  .short_caption = Write full command line
  .enum = Help
  .expert_level = 0
  .input_priority = 0
  .input_priority_if_present = 0
  .input_priority_if_only = False
  .help = Help
  .short_caption = Help
```

Correlation of map and model (deprecated, use MapCorrelations)

Author(s):

Tom Terwilliger, Tom Terwilliger

Purpose

get_cc_msz_pdb is a command line tool for obtaining the origin of a PDB file using sample group comments or a specified reflections file and calculating a map, obtaining the correlation of model and map, and analyzing the correlation for each residue.

Usage

How get_cc_msz_pdb works:

get_cc_msz_pdb calculates a model map based on the supplied PDB file. First uses MOSFLM to find the origin and cell parameters for the reflections file (if not specified) and then uses phenix.fmodel to calculate a model map and map coefficients (or use .mtz file). The map is sampled at the grid points in the map. A mask is calculated around the model using the radius specified (default 3 A). The map is then modified by setting values inside the mask equal to the average of values in and in shell around each sampled point.

The model is then shifted by one grid point in each direction and the correlation calculated.

By default model density is calculated using the atom types, occupancies and isotropic thermal factors (B-values) supplied in the PDB file. If you specify

-ignore_b

then all overall B is set to an increment of 0 (value for each atom beyond 20 the increment will be added to the value in the PDB file, after adjusting B-factors proportional to inverse mss-squared).

-ignore_occ

sets all occupancies to 1.

The correlation is then calculated for each residue (or specified residues) and saved in the B-factor field of the output file.

Example:

```
get_cc_msz_pdb model.pdb
```

Running the get_cc_msz_pdb command lines from the command line also can type:

```
phenix.get_cc_msz_pdb map_coeffs.mtz -ignore_b=yes
```

Alternatively, if you have a map in CCP4 format (from your map file), you will need to tell get_cc_msz_pdb what it was (MTZ file or ccp4 map). CCP4 map is the default:

```
phenix.get_cc_msz_pdb map_coeffs.mtz -ignore_b=yes
-map_type=ccp4 -ccp4_map=map.ccp4
```

Possible Problems

Specific limitations and problems:

The option to use phenix.fmodel to get cc_msz_pdb uses some extra conformers, because the CC values calculated by phenix.fmodel are slightly different than those from the MOSFLM file when CC statistics are used to calculate model density. This model density is compared to the map from your input map coefficients in the calculation of the correlation. Using the extra conformers allows the model density to better match the scaling seems the density obtained in area away from Group atoms.

Alternatively, if you have a map in CCP4 format (from your map file), phenix.fmodel the correlation coefficient (and map to give the correlation) using the scaling thermal parameters and excluding only the reflections present in the mtz file. Use the -ignore_b option if you want to ignore the values.

Example:

```
phenix.get_cc_msz_pdb map_coeffs.mtz -ignore_b=yes
-map_type=ccp4 -ccp4_map=map.ccp4
```

These defaults were changed so that the correlation values obtained by default is a close where to origin shift. Alternatively, if you have a map in CCP4 format (from your map file), phenix.fmodel the correlation coefficients and CC-F was from the PDB file and then determining the correlation between these two.

List of all available keywords

```
get_cc_msz_pdb
  pdb_file_name = None
  pdb_extension = None
                  Use this if extension is unusual.
                  Any recognized extension and pdb_extension is special in that when
                  reading a file with pdb_extension set to NONE or to a string that
                  does not end in pdb_extension the file will be read as a pdb file
                  if it can be read as a pdb file. Otherwise it will be read as a
                  PHENIX AUTO NAMED FORMAT FILE if it can be read as a PHENIX AUTO
                  NAMED FORMAT FILE. Otherwise it will be read as a pdb file.

  mtz_in = None   .mtz or .mtz.gzip map file
  ccp4 = None     .ccp4 or .map or .ccp4 or .map.gzip map file
                  Note: ccp4 and mtz cannot be specified together. If ccp4 and mtz
                  are specified, the first one in the command line will be used.

  ccp4_map_suffix = .ccp4
                  Suffix for ccp4 files to be read in if no suffix is specified
                  (default: .ccp4 or .map or .ccp4 or .map.gzip)

  resolution = None   High-resolution limit for map calculation

  use_phi_with_ccp4_map = False
                  Use phi values from ccp4 map in calculation if ccp4 map is read in

  sym = None      Space group for map calculation (if not specified or default is P1)

  mtz_labels = None   Labels for mtz file (comma-separated, for example
                  -mtz_labels=fobs,sigfobs,rfree,phi,fom,hla,hlb,hlc,hlm
                  -mtz_labels=fobs,sigfobs,rfree,fom,hla,hlb,hlc,hlm
                  -mtz_labels=fobs,sigfobs,rfree,hla,hlb,hlc,hlm
                  -mtz_labels=fobs,sigfobs,rfree,hla,hlb,hlc,hlm,phi,fom
                  -mtz_labels=fobs,sigfobs,rfree,phi,fom
                  -mtz_labels=fobs,sigfobs,rfree
                  -mtz_labels=fobs,sigfobs,rfree,hla,hlb,hlc,hlm,phi,fom
                  -mtz_labels=fobs,sigfobs,rfree,hla,hlb,hlc,hlm,phi,fom,hla,hlb,hlc,hlm
                  -mtz_labels=fobs,sigfobs,rfree,phi,fom,hla,hlb,hlc,hlm
                  -mtz_labels=fobs,sigfobs,rfree,phi,fom,hla,hlb,hlc,hlm
```

```
  action: true                    # Action output
  quiet: false                    # Suppresses informational messages
  quote_char: '"'                 # Quote character
  force: false                    # Force write of problems
  debug: false                    # Debugging output
  verbose: false                  # Verbose output with extra parameter names
  record_separator: "\n"          # The record separator character to use when outputting multi-line records. Defaults to "\n" (newline). Common alternatives: "\r\n" (Windows), "\r" (old Mac), "\0" (null), "\t" (tab), "|" (pipe), "~" (tilde)
  job_size: 5000                  # Job size for MPMD mode. Set to 0 to disable MPMD
  mpmd: false
  mpmd_output_format: "%rid:%jid:%stdout:%stderr:%exit:%time:%cmd:%host:%start:%finish:%pid:%signal:%kmg:%vmg:%tmg:%kcpu:%vcpu:%tcpu:%rss:%vsz:%swap:%mem:%io:%iop:%ior:%iow:%maj:%min:%pgin:%pgout:%vol:%inv:%nice:%prio:%sys:%usr:%tsys:%tusr:%cpu:%wait:%ncpu:%nhost:%hostlist:%mem:%cmd:%jobid:%jobpid:%jobcmd:%jobhost:%jobstart:%jobfinish:%jobexit:%jobsignal:%jobstat:%jobtime:%queue:%pjobid:%pjobpid:%pjobcmd:%pjobhost:%pjobstart:%pjobfinish:%pjobexit:%pjobsignal:%pjobstat:%pjobtime:%pqueue:%pjobmem:%pjobcpu:%pjobmem:%pjobio:%pjobiop:%pjobior:%pjobiow:%pjobmaj:%pjobmin:%pjobpgin:%pjobpgout:%pjobvol:%pjobinv:%pjobnice:%pjobprio:%pjobsys:%pjobusr:%pjobtsys:%pjobtusr:%pjobcpu:%pjobwait:%pjobncpu:%pjobnhost:%pjobhostlist:%pjobmem:%pjobcmd:%pjobjobid:%pjobjobpid:%pjobjobcmd:%pjobjobhost:%pjobjobstart:%pjobjobfinish:%pjobjobexit:%pjobjobsignal:%pjobjobstat:%pjobjobtime:%pjobjobqueue:%pjobjobmem:%pjobjobcpu:%pjobjobmem:%pjobjobio:%pjobjobiop:%pjobjobior:%pjobjobiow:%pjobjobmaj:%pjobjobmin:%pjobjobpgin:%pjobjobpgout:%pjobjobvol:%pjobjobinv:%pjobjobnice:%pjobjobprio:%pjobjobsys:%pjobjobusr:%pjobjobtsys:%pjobjobtusr:%pjobjobcpu:%pjobjobwait:%pjobjobncpu:%pjobjobnhost:%pjobjobhostlist:%pjobjobmem:%pjobjobcmd:%pjobjobjobid:%pjobjobjobpid:%pjobjobjobcmd:%pjobjobjobhost:%pjobjobjobstart:%pjobjobjobfinish:%pjobjobjobexit:%pjobjobjobsignal:%pjobjobjobstat:%pjobjobjobtime:%pjobjobjobqueue:%pjobjobjobmem:%pjobjobjobcpu:%pjobjobjobmem:%pjobjobjobio:%pjobjobjobiop:%pjobjobjobior:%pjobjobjobiow:%pjobjobjobmaj:%pjobjobjobmin:%pjobjobjobpgin:%pjobjobjobpgout:%pjobjobjobvol:%pjobjobjobinv:%pjobjobjobnice:%pjobjobjobprio:%pjobjobjobsys:%pjobjobjobusr:%pjobjobjobtsys:%pjobjobjobtusr:%pjobjobjobcpu:%pjobjobjobwait:%pjobjobjobncpu:%pjobjobjobnhost:%pjobjobjobhostlist:%pjobjobjobmem:%pjobjobjobcmd:%pjobjobjobjobid:%pjobjobjobjobpid:%pjobjobjobjobcmd:%pjobjobjobjobhost:%pjobjobjobjobstart:%pjobjobjobjobfinish:%pjobjobjobjobexit:%pjobjobjobjobsignal:%pjobjobjobjobstat:%pjobjobjobjobtime:%pjobjobjobjobqueue:%pjobjobjobjobmem:%pjobjobjobjobcpu:%pjobjobjobjobmem:%pjobjobjobjobio:%pjobjobjobjobiop:%pjobjobjobjobior:%pjobjobjobjobiow:%pjobjobjobjobmaj:%pjobjobjobjobmin:%pjobjobjobjobpgin:%pjobjobjobjobpgout:%pjobjobjobjobvol:%pjobjobjobjobinv:%pjobjobjobjobnice:%pjobjobjobjobprio:%pjobjobjobjobsys:%pjobjobjobjobusr:%pjobjobjobjobtsys:%pjobjobjobjobtusr:%pjobjobjobjobcpu:%pjobjobjobjobwait:%pjobjobjobjobncpu:%pjobjobjobjobnhost:%pjobjobjobjobhostlist:%pjobjobjobjobmem:%pjobjobjobjobcmd:%pjobjobjobjobjobid:%pjobjobjobjobjobpid:%pjobjobjobjobjobcmd:%pjobjobjobjobjobhost:%pjobjobjobjobjobstart:%pjobjobjobjobjobfinish:%pjobjobjobjobjobexit:%pjobjobjobjobjobsignal:%pjobjobjobjobjobstat:%pjobjobjobjobjobtime:%pjobjobjobjobjobqueue:%pjobjobjobjobjobmem:%pjobjobjobjobjobcpu:%pjobjobjobjobjobmem:%pjobjobjobjobjobio:%pjobjobjobjobjobiop:%pjobjobjobjobjobior:%pjobjobjobjobjobiow:%pjobjobjobjobjobmaj:%pjobjobjobjobjobmin:%pjobjobjobjobjobpgin:%pjobjobjobjobjobpgout:%pjobjobjobjobjobvol:%pjobjobjobjobjobinv:%pjobjobjobjobjobnice:%pjobjobjobjobjobprio:%pjobjobjobjobjobsys:%pjobjobjobjobjobusr:%pjobjobjobjobjobtsys:%pjobjobjobjobjobtusr:%pjobjobjobjobjobcpu:%pjobjobjobjobjobwait:%pjobjobjobjobjobncpu:%pjobjobjobjobjobnhost:%pjobjobjobjobjobhostlist:%pjobjobjobjobjobmem:%pjobjobjobjobjobcmd:%pjobjobjobjobjobjobid:%pjobjobjobjobjobjobpid:%pjobjobjobjobjobjobcmd:%pjobjobjobjobjobjobhost:%pjobjobjobjobjobjobstart:%pjobjobjobjobjobjobfinish:%pjobjobjobjobjobjobexit:%pjobjobjobjobjobjobsignal:%pjobjobjobjobjobjobstat:%pjobjobjobjobjobjobtime:%pjobjobjobjobjobjobqueue:%pjobjobjobjobjobjobmem:%pjobjobjobjobjobjobcpu:%pjobjobjobjobjobjobmem:%pjobjobjobjobjobjobio:%pjobjobjobjobjobjobiop:%pjobjobjobjobjobjobior:%pjobjobjobjobjobjobiow:%pjobjobjobjobjobjobmaj:%pjobjobjobjobjobjobmin:%pjobjobjobjobjobjobpgin:%pjobjobjobjobjobjobpgout:%pjobjobjobjobjobjobvol:%pjobjobjobjobjobjobinv:%pjobjobjobjobjobjobnice:%pjobjobjobjobjobjobprio:%pjobjobjobjobjobjobsys:%pjobjobjobjobjobjobusr:%pjobjobjobjobjobjobtsys:%pjobjobjobjobjobjobtusr:%pjobjobjobjobjobjobcpu:%pjobjobjobjobjobjobwait:%pjobjobjobjobjobjobncpu:%pjobjobjobjobjobjobnhost:%pjobjobjobjobjobjobhostlist:%pjobjobjobjobjobjobmem:%pjobjobjobjobjobjobcmd:%pjobjobjobjobjobjobjobid:%pjobjobjobjobjobjobjobpid:%pjobjobjobjobjobjobjobcmd:%pjobjobjobjobjobjobjobhost:%pjobjobjobjobjobjobjobstart:%pjobjobjobjobjobjobjobfinish:%pjobjobjobjobjobjobjobexit:%pjobjobjobjobjobjobjobsignal:%pjobjobjobjobjobjobjobstat:%pjobjobjobjobjobjobjobtime:%pjobjobjobjobjobjobjobqueue:%pjobjobjobjobjobjobjobmem:%pjobjobjobjobjobjobjobcpu:%pjobjobjobjobjobjobjobmem:%pjobjobjobjobjobjobjobio:%pjobjobjobjobjobjobjobiop:%pjobjobjobjobjobjobjobior:%pjobjobjobjobjobjobjobiow:%pjobjobjobjobjobjobjobmaj:%pjobjobjobjobjobjobjobmin:%pjobjobjobjobjobjobjobpgin:%pjobjobjobjobjobjobjobpgout:%pjobjobjobjobjobjobjobvol:%pjobjobjobjobjobjobjobinv:%pjobjobjobjobjobjobjobnice:%pjobjobjobjobjobjobjobprio:%pjobjobjobjobjobjobjobsys:%pjobjobjobjobjobjobjobusr:%pjobjobjobjobjobjobjobtsys:%pjobjobjob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```

get_pdb_validation_report

Advanced Beamline Monitoring & Remote Diagnostic

phenix.get_pdb_validation_report

Description

The tool to fetch validation reports from Grading validation. Only mmCIF format is supported for models and structure factors. Only PDF format for XY plots. PDB internal plots in XY format are not currently supported. If validation completed successfully, a validation report in pdf and XY format will appear on hard drive.

Note: Validation reports are available for a subset of PDB structures. Structures must have been processed by wwPDB validation pipeline and released in PDB archive. The tool will return a message on STDOUT if validation report is not available for requested structure.

Note: running the tool again with flag will create a new session on the validation server, not require about a previous one.

WARNING

Please do not spam your model and data to RCSB servers for processing. Please refer to their privacy policy for details.

https://www.rcsb.org/pdb/static/privacy

Command line usage examples

```
phenix.get_pdb_validation_report --help=yes --help=no --help=all
phenix.get_pdb_validation_report session_id=1ifc4ZeV7EC6QeeGFFHm.PeaFQ0db3Ic3uzMMq
phenix.get_pdb_validation_report model=pf structure_factors=pf
phenix.get_pdb_validation_report model=pf map.ccp4
```

GUI

The graphical user interface is currently available in the "PDB Validation" section. Very few GUI self-remember options are available. Please use command line version if you need to keep the results in certain folder. When the results are fetched, the resulting pdf and XY plot appear in phenix.find.

List of all available keywords

```
help=yes                    Prints a brief list the keywords, or options
help=keywords               Prints brief help for the keywords, or options
session_id = None           Session ID for the get_validation_report
model = None                Model file for validation
map_file = None             Map file for validation
mode = None                 Mode: XML, CIF, PDF, XY, ALL, CLEAN, CLEANALL, CLEANCIF, CLEANXY
  pdf=yes                   Get pdf report
  xy=yes                    Get XY report
  all=yes                   Get all reports
```

PHENIX(PHENIX) (WHERE THE POWER DWELLS)

Phenix *Python Hierarchical Environment for Integrated Crystallography*

Guess location of molecular centers in a map with **guess_molecular_centers**

Author(s)

- Jack Greenhow

Purpose

guess_molecular_centers is a tool to identify potential locations of molecules in an electron density map.

Uses

How **guess_molecular_centers** works:

guess_molecular_centers finds potential molecular centers in the density map by finding local maxima of the local CC density. You can specify the number of local maxima and a minimum local CC density.

Output files from **guess_molecular_centers**

guess_molecular_centers.pdb A PDB file with pseudo-atoms marking the locations of centers of your density map.

Examples

Standard use of **guess_molecular_centers**:

Running guess_molecular_centers is easy. From the command line you can type:

```
phenix.guess_molecular_centers map_coeffs.mtz
```

Possible Problems

- Sometimes the default settings will fail to recognize the lattice used for smoothing (smoothing_lattice). If you know that the smoothing lattice, you can try loading the mask by changing it_lattice_file.
- Large maps can take a long time.

Literature

1. **Finding microcrystallographic symmetry in density maps of macromolecular structures.** TJ. Greenhow, P. Zwart, P. D. Adams, N. W. Moriarty.

List of all available keywords

```
guess_molecular_centers
  input_files
    map_file .type = Map                  Map file with coefficients for a map
    mask .type = Mask                     Optional mask file to limit the calculation. This is optional if
                                          you specify the mask_file and map_file. Only points inside the mask
                                          will be considered. Note that the mask should contain the same
                                          grid as the input map(s). Note that the mask should contain only
                                          zero and one.
  output_files
    local_corr_map_file .type = Map       Map file local corr is written. Values are Map1 * Map2 * CC (if
                                          local_cc_cutoff is set, then values below local_cc_cutoff are set
                                          to zero). Note that this map is always shifted to the origin.
                                          Output mask will be in the same shifted cell.
    pdb_out .type = pdb                   Output PDB file
    log .type = output logfile            Output log file
    prefix .def = guess_molecular_centers
  directories
    temp_dir .type = Path .multi = True   Optional temporary work directory
    output_dir .type = Path               Output directory (data files will be written
  find_centers
    n_centers .type = int .value_min = 1  Number for searching peaked density to find centers (leave a smaller
                                          value if not enough centers)
    n_centers_final .type = int           Number of centers to keep
    n_centers_step .type = int            Step number of centers and find smoothing lattice until the number
                                          of centers is n_centers_final (if n_centers_step is zero, n_centers
                                          is used)
  cluster_info
    cluster_radius .type = float          Cluster radius (used for map calculation)
    cluster_fraction .type = float        Cluster fraction
  control
    verbose .type = bool                  Verbose output
    nproc .type = int                     None array of problems
    write_files .type = bool              Write output files
    dry_run .type = bool                  Dry run
    overwrite_numbered_files .type = bool Over ride or not files numbered with a number (if overwrite
                                          false, then new files will be written with a number that is one
                                          higher than any existing number in output_dir). If the root
                                          filename is not specified, then a file with a random
                                          hexadecimal filename will be written.
```

PhenixOnline *Python-based Hierarchical Environment for Integrated Crystallography*

Guided Ligand Replacement

Contents

- Overview
- Input files
- Output files
- Examples
  - Example 1
  - Example 2
- References
- List of all available keywords

Authors: Ralf W. Grosse-Kunstleve & Jiri Jaroszewski

Overview

The Guided Ligand Replacement (GLR) module is intended to facilitate ligand placement when the is a close ligand-containing structure available in the same crystal form. The module takes a ligand-containing structure and a single-chain protein sequence and produces a new ligand-protein complex (coordinates and reflections). It is essentially a wrapper around the phenix.ligand_pipeline and phenix.refine programs with a few additional options.

The Guided Ligand Replacement (GLR) tool is designed to use prior knowledge from a previously fit ligand to guide the search for a new ligand in a related "target" protein. The similarity required between the pair of ligands can be as little as a few atoms.

The process can optionally also use a custom pdb. The ligands are matched using the electronic ligand interpretation (ELI) tool. The ligand in the custom pdb is matched against the ligand in the input pdb file. If a ligand is found, a Ligand Bond Restraint (LBRG) is generated and will be used during refine.

Usage

Usage:

```
phenix.guided_ligand_replacement target.pdb
  ligand_pdb_file_name=ligand_in_other_structure.pdb
  ligand_code_in_other_structure=LIG
  target_protein_sequence=protein.seq
  target_ligand_code=LIG
  output.prefix=my_output_prefix
  output.overwrite=True
  output.write_intermediate_files=True
  output.write_log_file=True
  output.write_ligand_bond_restraints=TRUE
```

Input files

See specifying a number of inputs and also has some options, all of which are provided using the pro formatted input file:

- **guide_pdb_file_name**: Name of the PDB file for the structure of the reference protein-ligand complex. This structure will be used to generate a ligand restraint file and to align the target protein sequence with the reference protein to identify equivalent residues. Optional keywords: guide_pdb_file_name=pdb_with_ligand.pdb
- **target_pdb_file_name**: Name of the PDB file for the target protein structure. This structure is expected to be apo structure from molecular replacement after rigid body refinement.
- **map_coeffs_file_name**: Name of the input reflection file that will be used in refine and to generate the difference map. The input reflection file can be either in mtz or sca format. If the file contains more than one set of available map coefficients, the first (sorted alph. by labels) will be used. Optional keywords: map_coeffs_file_name=my_data.mtz, map_coeffs_file_name=my_data.sca
- **output.prefix**: Prefix for output files. Default: output

The input to the Guided Ligand Replacement tool may be provided as a single PDB file or both of the following pdb parameters can be used:

- **target_pdb_file_name**: this is a file containing chain(s) of interestion about the ligand.
- **ligand_pdb_file_name**: this is the ligand-containing PDB file for the PDB about. If not supplied, the ligand will be searched for in the target_pdb_file_name file.
- **ligand_code**: the ligand code from the PDB Chemical Components so that restraints and coordinates can be generated.

Optional inputs include:

- **ligand_selection_in_guide_model**: Ligand PDB selection expression to identify the ligand in the guide model. Optional keywords: ligand_selection_in_guide_model="resseq 1 and chain A", default is to find a single ligand-containing model in ligand code or unless there is only one ligand in the guide model.
- **replace_ligand_in_guide_pdb_file_name=True/False**: By default, this parameter is set to False. If set to True, the ligand in the guide model will be replaced with the ligand found in the target structure. Default: False. Optional keywords: replace_ligand_in_guide_pdb_file_name=True
- **output.write_intermediate_files**: Optional keywords:

```
  If the first step of the ligand is guided search is set to GUIDE
  then the intermediate files are written out.

  If the current ligand is selected as the guide ligand and if
  output.write_intermediate_files=True then the
```

- **phenix.superpose_pdbs**: Pro allows selection of the same parameters as in the standalone program.

Output files

The program will generate a PDB file with the fit ligand.

Examples

Example 1

The reference PDB structure, 5R3A, and the reference ligand, LVB, is used to place the target ligand, LVB, in the target PDB structure 5R3C.

```
phenix.guided_ligand_replacement
  target_pdb_file_name=5R3C.pdb
  guide_pdb_file_name=5R3A.pdb
  ligand_code=LVB
  map_coeffs_file_name=5R3C.mtz
  output.prefix=5R3C_with_5R3A_ligand
  output.overwrite=True
```

Example 2

In all of the above examples, the input can be provided through a PKG file.

```
phenix.guided_ligand_replacement ligand.pro
```

References

- **Electronic ligand interpretation for pdb structures: the guided ligand replacement method**, G.F. Ove, J.M. Jaroszewski, Jiri Jaroszewski, R.W. Grosse-Kunstleve, P. Bunkóczi, P. Adams, T. Terwilliger, Acta Crystallographica D, 2022, 78, 1-9, https://doi.org/10.1107/S2059798321011895
- **phenix.ligand Pocket and Optimization Workbench (LPOW) a tool for ligand coordinate and restraint optimization**, Jiri Jaroszewski, R.W. Grosse-Kunstleve, Ralf W. Grosse, Acta Crystallog. D 77, 1-11 (2021), https://doi.org/10.1107/S2059798320013955

List of all available keywords

```
guide_ligand_selection
  guide_ligand_selection=None
  ligand
    ligand=None
      guide_pdb_file_name=None      Guide PDB filename containing protein model and ligand that can
                                    assist the placement of the ligand into the apo model
      protein_pdb_file_name=None    The file containing protein pdb which the ligand will be fit.
                                    Optional keywords: protein_pdb_file_name=protein.pdb
      ligand_code=None              Ligand code for the ligand to be placed in the target model
                                    Optional keywords: ligand_code=LIG
      pdb_file_name=None            Ligand-containing PDB filename
      ligand_selection=None         Ligand selection
      map_coeffs_file_name=None     Map coefficients file a difference if the apo model
                                    Optional keywords: map_coeffs_file_name=my_data.mtz
      ligand_selection_in_guide_model=None  Ligand selection in the guide model. If not
                                    specified, all ligands will be used. Optional keywords: ligand
                                    selection=resseq 1 and chain A
      replace_ligand_in_guide_pdb_file_name=False  Replace the ligand in the guide model. This
                                    option works primarily in the GUIDE-TF-FOR-LIGAND-SEARCH.
  ligand_code=None
  pdb_file_name=None
  output
    prefix=None                     Default for output filenames
    log_level=None                  DEV-ONLY PRAGMA-ADVI: set level of verbose log
  superpose_pdbs
    pdb_file_name=None
      pdb_file_name_ignore_1=None
      pdb_file_name_ignore_2=None
      pdb_file_name_ignore_3=None   DEV-ONLY PRAGMA-ADVI: Max file with model that will be fit to pdb_file_name_protein
      pdb_file_name_protein=None    DEV-ONLY PRAGMA-ADVI: Protein file to superpose with the pdb_file_name
    output
      prefix=superpose_pdbs         Prefix for output files
      write_superposed_pdbs=True    Write superposed pdbs
      write_log_file=True           Write log file
      log_file_name=superpose.log   Name of log file
      write_rotation_matrices=False Write rotation matrices
    superpose
      chain_id=None                 Chain ID
      pick_ligand_atoms=True        Pick ligand atoms
      ligand_selection=None         Ligand selection
      ignore_hydrogens=True         Ignore hydrogens
      ignore_ligand_atoms=False     Ignore ligand atoms
    verbose
      verbose=True                  Verbose
      debug=False
    parallel
      nproc=1                       Number of processors
  target_pdb_file_name=None         Target PDB file
  target_protein_sequence=None      Target protein sequence
  target_ligand_code=None           Target ligand code
  map_coeffs_file_name=None         Map coefficients file
  output
    prefix=output                   Prefix for output files
    overwrite=False                 Overwrite existing files
    write_intermediate_files=False  Write intermediate files
    write_log_file=True             Write log file
    log_file_name=guide.log         Name of log file
    write_ligand_bond_restraints=False  Write ligand bond restraints
  ligand_pdb_file_name=None         Ligand PDB file
  ligand_code=None                  Ligand code
  superpose_pdbs
    pdb_file_name=None
      pdb_file_name_ignore_1=None
      pdb_file_name_ignore_2=None
      pdb_file_name_ignore_3=None
      pdb_file_name_protein=None
    output
      prefix=superpose_pdbs
      write_superposed_pdbs=True
      write_log_file=True
      log_file_name=superpose.log
      write_rotation_matrices=False
    superpose
      chain_id=None
      pick_ligand_atoms=True
      ligand_selection=None
      ignore_hydrogens=True
      ignore_ligand_atoms=False
    verbose
      verbose=True
      debug=False
    parallel
      nproc=1
  verbose
    verbose=True
    debug=False
  parallel
    nproc=1
```

hoion_geometry_validation

Phenix *Python based Hierarchical Environment for Integrated Crystallography*

Evaluating a model with Hoion geometry validation

Author(s)

Tom Terwilliger, geometry validation; James Holton (Python coding by Tom Terwilliger)

Purpose

Estimates geometric quality of a model.

How hoion_geometry_validation works:

This tool summarizes the geometric quality of a model by calculating peptide energies (square of the sides of a triangle formed by the Cα atoms of two peptide bonds), Ramachandran energies (distance from the center of the Ramachandran plot), Rot and Cβ outlier fraction of residues, the mean energy and standard deviation of bond and angle deviations, the number of cis-peptides, the number of Cβ deviations, the number of clashes, the fraction of bad bond and angle deviations, and the number of Cα deviations. The energy values are scaled so that the standard deviation of any one energy, energy squared is one. Cα and Rotamer by measuring these research, Cβ and clashes are based on the Molprobity definitions, and the other energies are based on the Ramachandran plot and the Phenix bond and angle deviations.

The output looks like this (for a set of randomly perturbed 500 residues of 1ubq). The metrics used are:

```
Ramachandran Deviation of 20 positions from ideal (%)
Rotamer Deviation of 20 positions (%)
Peptide  Mean=0.000 Sigma=0.000 Deviation=0.000
Cbeta    Mean=0.000 Sigma=0.000 Deviation=0.000
Bond     Mean=0.000 Sigma=0.000 Deviation=0.000
Angle    Mean=0.000 Sigma=0.000 Deviation=0.000
Clashes  Mean=0.000 Sigma=0.000 Deviation=0.000
Calpha   Mean=0.000 Sigma=0.000 Deviation=0.000
Cis-peptides 0 out of 20 (0.00%)
Ramachandran Mean=0.000 Sigma=0.000 Deviation=0.000
Rotamer Mean=0.000 Sigma=0.000 Deviation=0.000
Bad bond lengths 0 out of 20 (0.00%) Bad bond angles 0 out of 20 (0.00%)
Bad Cbeta 0 out of 20 (0.00%) Bad Calpha 0 out of 20 (0.00%)
Bad Rotamer 0 out of 20 (0.00%) Bad Ramachandran 0 out of 20 (0.00%)
```

Estimate of expected energy for ideal structure

This tool estimates the expected energy for a structure that has all bonds, angles, etc. distributed as in the Molprobity or Phenix geometry restraints definitions of ideal structure. The energy is calculated by adding the square of the deviation of every function value from its ideal value. The energy is estimated by adding these values for all of the functions that are used in the Molprobity or Phenix geometry restraints. The standard deviation of the contribution from each term is estimated by the square root of the number of terms times 0.25 (so the standard deviation of the ideal deviations). The sampling provides a check on this estimate.

Estimate of ratio of deviations to sigmas

This tool estimates the overall ratio of deviations to sigmas in three steps:

1. Calculate the standard deviation of the deviations from ideal for the functions used in the Phenix or Molprobity geometry restraints. Calculate the standard deviation of the deviations from ideal for the functions used in the Phenix or Molprobity geometry restraints. Calculate the ratio of these two standard deviations. This ratio is estimated by adding these two standard deviations and dividing by the standard deviation of the ideal deviations. The sampling provides a check on this estimate.

Estimate of ratio of deviations to sigmas

This tool estimates the overall ratio of deviations to sigmas in three steps:

1. Calculate the standard deviation of the deviations from ideal for the functions used in the Phenix or Molprobity geometry restraints. Calculate the standard deviation of the deviations from ideal for the functions used in the Phenix or Molprobity geometry restraints. Calculate the ratio of these two standard deviations. This ratio is estimated by adding these two standard deviations and dividing by the standard deviation of the ideal deviations. The sampling provides a check on this estimate.

Then the RS-TS percentile of values of deviations/sigmas is ranked from a Gaussian distribution. This percentile provides a measure of how unusual the deviations are. A value of 0 means the value is lower than 0.01 of the RS-TS percentile value, and a standard deviation of the value of deviations/sigmas.

Comparing two models

If you want to be quick and check whether model A is better than B-phi, you can supply both models to hoion_geometry_validation. The output will be the same as for one model, but it will also provide scores for A-phi and B-phi (only not just the standard parameters, but all ideaselfs values of these parameters). The output will also provide the number of cases where the deviation from ideal is better for model A than for B, the number of cases where the deviation from ideal is better for B than for A, and the number of cases where the difference in deviation from ideal is equal for A and B (within 0.01 standard deviations).

You can supply a list of models as well (or a model and a set of other_models), and each will be compared to the first model in the list.

Uses

You can use hoion geometry validation to compare models for the same structure and identify which has fewer bad geometry features.

You can use the expected energy to see if your structure has more than you about what a expected based on ideal model generally and unusualness.

You can use the estimate of ratio of deviations to sigmas to further examine whether the deviations from ideally in your structure are about what is expected based on the supplied weights in geometry refine.

Comparing a series of models to see how each corresponds to the first model.

Examples

Standard run of hoion_geometry_validation:

Reading model geometry, coordinates & data. Find the connected lines and run type:

```
phenix.hoion_geometry_validation model.pdb
```

where model_a.pdb is the model you would like to evaluate.

Possible Problems

If your structure has hydrogen positions that do not match those expected by Phenix, you can ignore them or all hydrogen positions in your structure will be ignored. If this is unusual, an unexpected flag. Alternatively you can delete their positions with keep_hydrogens=false.

If you want to ignore just hydrogen positions in Phenix mechanics you can specify ignore_any_h_contacts=true.

If you want to ignore hydrogen positions in Phenix mechanics you can specify ignore_any_h_contacts=true. If you want to include all bonds involving hydrogen, specify bond_weight_with_h=true.

Literature

The method is described at https://doi.org/10.1107/S0907444909047507 Phenix

Additional information

List of all available keywords

```
model = None                          input PDB file
data = None                           input reflection data
get_selected_model_only = False       Consider selected residue scores or particular to overall score
get_selected_model_score = None       Residue selection for scoring
write_cbeta_in_ca_pdb_file=False      Write Cbeta
                                      Write Cbeta as Ca in a pdb file (Ca is where Cb is here) (takes
                                      PDB number of clashes to CaB energy score)
read_cbeta_pdb = None                 Read Cbeta from a pdb file (Ca is where Cb is here)
write_cbeta_pdb_file = None           Write Cbeta to a pdb file
write_cbeta_pdb_file_min_deviation=0.5
                                      Write Cbeta to a pdb file only if deviation is at or above this
                                      value
include_bad_cbeta_pdb=True            Include bad cbeta (not in rotamer or at a cis-peptide) in pdb
                                      file (if write_cbeta_pdb_file is set)
keep_hydrogens = True                 If set, keep bond hydrogens, but add any necessary (using H-
                                      bond) hydrogens to the model (default is to remove hydrogens)
ignore_hydrogen_in_ambiguous = True   If set, ignore H-bond scores in ambiguous
ignore_any_h_contacts = True          If set, ignore H-bond in Ramachandran
                                      Ignore any H-bond contacts involving H atoms
ignore_water_h_bonds = True           If set, ignore H-bond contacts involving H atoms
                                      If set, ignore H-bond contacts involving H atoms
                                      Number of bins for Ramachandran
overall_bond_weight = None            Optional scale of energy
bond_weight = None                    Scale for bond energy
angle_weight = None                   Scale for Cb deviation
clashscore_target_per = 0             Ideal clashscore in clashes/1000a generated for clashscore report
clashscore_target_per_sigma = 0       Sigma for ideal clashscore in clashes/1000a generated for clashscore
cbeta_deviation_weight = None         Extra weight factor for cbeta deviation energies (pdb mode)
cbeta_deviation_sigma = None          Sigma for cbeta deviation energies (pdb mode)
                                      Sigma for cbeta deviation energies (pdb mode)
cbeta_deviation_min_sigma = None      Minimum sigma for cbeta deviation energies (pdb mode)
                                      Minimum sigma for cbeta deviation energies (pdb mode)
                                      Number of cbeta deviations
                                      Number of cbeta deviations
model_weight = None                   Weight model energy
score_only_with_weight = None         Score and show without weight
include_cbeta = True                  Include cbeta deviation in pdb mode
include_rotamer = True                Include rotamer score for structure (not model score)
sigma = 0.25                          Sigma for ideal bond and angle deviations
sigma_squared = 0.0625                Sigma squared
                                      Sigma squared
                                      Sigma squared
                                      
```

Phenix *Python-based Hierarchical Environment for Integrated Xtallography*

phenix.reduce: tool for adding hydrogens to a PDB model

Purpose:

phenix.reduce is a command line tool for adding hydrogens to a PDB structure file. Hydrogens are added in chemically sensible sites optimized for the orientations of all the polar, flip-capable, hydroxyl, and thiol groups, and the positions of all the hydrogen atoms are optimized for maximum H-bonding and minimum steric overlap. A description of the algorithm is provided. The program is described in Word et al (1999). The program is free for the asking. For more information see http://kinemage.biochem.duke.edu/software/reduce.php

How to run:

phenix.reduce is run from the command line:

```
phenix.reduce [opts.file] [pdb.pdb]
```

To get information about command line options type:

```
phenix.reduce -help
```

or for a longer list:

```
phenix.reduce -v
```

Hydrogens in references:

Please refer to phenix online documentation to see how hydrogen atoms are used in structure refinement.

Phenix

Action-based Recursive Efficiencies for Enzymatic Reliquefy

Hybrid Substructure Search

Contents

- Authors
- Hy36 overview
- A new powerful and parallel Hybrid Substructure Search (HyS2)
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- Trying a search without automatic termination
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- Trying likelihood-based searching with direct methods
- Searches for heavy-atom cluster compounds
- Notes
- Auxiliary programs
- phenix.anome
- References
- List of all available keywords

Authors

Ralf Grosse-Kunstleve, Paul Adams, Randy Read, Gabor Bunkóczi, Tom Terwilliger

Hy36 overview

The Hybrid 36 (Hy36) extension to the Protein Data Bank (PDB) format provides a highly backwards compatible way to write and read more than 99999 atoms and 9999 residues per PDB file. Hy36 supports all features of the reference file format and analyses all available datasets in a given reflection file to decide which of these is most suitable for output. Hy36 is used by default in the Phenix software suite and can be enabled in other software by a variety of standard ways (e.g. by the CCP4 Libraries). The main reason for a suitable Hy36 implementation is that it allows:

- Direct binary reflection interpretation followed by
- Automatic data preparation (including automatic termination)
- and finally Direct Methods or Molecular Replacement followed by
- automatic model building and refinement
- automatic termination detection

The ease of use of the Phenix software suite is expected in a variety of file formats suitable for frequently used phasing and density modification pathways.

The core search procedure is applicable to both enumerated diffraction and reconstructed replacement problems (Grosse-Kunstleve & Adams, 2002). The search procedure is also applicable to Patterson-based searches, but this is not discussed in this document.

A new powerful and parallel Hybrid Substructure Search (HyS2)

The Hybrid Substructure Search (HyS2) is a powerful and parallel implementation of the Shake-and-Bake (SnB) procedure (Weeks et al. 1994). The main differences between the two implementations are:

- HyS2 is parallel, SnB is not.
- HyS2 supports the Phase Ambiguity Resolution (PAR) procedure (Grosse-Kunstleve & Adams, 2002) and can therefore handle centrosymmetric data.
- HyS2 supports the Tangent Formula (TF) procedure (Karle & Hauptman, 1956) and can therefore handle centrosymmetric data.
- HyS2 supports the Minimal Function (MF) procedure (Hauptman, 1972) and can therefore handle centrosymmetric data.
- HyS2 supports the Difference Fourier (DF) procedure (Fujinaga & Read, 1987) and can therefore handle centrosymmetric data.
- HyS2 supports the Difference Patterson (DP) procedure (Sheldrick & Dauter, 1999) and can therefore handle centrosymmetric data.
- HyS2 supports the Difference Minimal Function (DMF) procedure (Hauptman, 1975) and can therefore handle centrosymmetric data.
- HyS2 supports the Difference Tangent Formula (DTF) procedure (Karle, 1989) and can therefore handle centrosymmetric data.
- HyS2 supports the Difference Phase Ambiguity Resolution (DPAR) procedure (Grosse-Kunstleve & Adams, 2002

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Python-based Hierarchical Environment for Integrated Xtallography

Phenix help chapters

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- Phenix.Refine: Refinement of protein and nucleic acid models with phenix.ncs_refine
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- Phenix.Refine: Refinement of protein and nucleic acid models with phenix.ncs_refine and phenix.hydrogen_refine
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- Phenix.Refine: Refinement of protein and nucleic acid models with phenix.real_space_refine
- Phenix.Refine: Refinement of protein and nucleic acid models with phenix.ncs_refine
- Phenix.Refine: Refinement of protein and nucleic acid models with phenix.hydrogen_refine
- Phenix.Refine: Refinement of protein and nucleic acid models with phenix.real_space_refine
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Phenix

Python based Hierarchical Environment for Integrated Xtallography

Automated Sgand Identification

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- Keywords for phenix.sgtoinfo
- Keywords for phenix.sgtoinfo

List of all available keywords

Note: In case search parameters in legal descriptions, the parameter prefixes (i.e. the bold text above the desired keyword) should be added to the keywords. For example,

- keyword: `name_contains`
- search-parameter-prefix: **`legal_`**

The specific number of scopes of the legal is the asymptotic unit.

- `search_parameters.name_contains`: (optional)

`legal_identifier`

- `id`: `Int64`
- `jurisdiction_id`: `Int64`
- `jurisdiction_name`: `Text`
- `jurisdiction_classification`: `Text`
- `legal_type`: `Text`
  - Enum: `"Act"`, `"Bill"`, `"Amendment"`, `"Motion"`, `"Resolution"`, `"Regulation"`, `"Order in Council"`, `"Proclamation"`, `"Manual"`, `"Policy"`, `"Publication"`, `"Other"`
- `legal_type_id`: `Int`
- `name`: `Text`
- `name_en`: `Text`
- `name_fr`: `Text`
- `scraped_tags`: `[Text]`
- `inst_identifier`: `Text`
- `inst_classification`: `Text`
- `inst_name`: `Text`
- `parliament_session`: `Text`
- `updated_at`: `Timestamp`
- `extra`: `{}`
- `latest_action_dt`: `Date`
- `latest_action_description`: `Text`
- `latest_motion`: `Text`
- `first_nation`: `Text`
- `abstract`: `Text`
- `other_titles`: `[{}]`
- `other_dates`: `[{}]`
- `related_bills`: `[{}]`
- `sources`: `[{}]`
- `sponsors`: `[{}]`
- `votes`: `[{}]`
- `extras`: `{}`
- `updated_at_1`: `Timestamp`
- `latest_action_dt_1`: `Date`
- `id_1`: `Int`
- `jurisdiction_id_1`: `Int`
- `jurisdiction_name_1`: `Text`
- `legal_type_id_1`: `Int`
- `name_1`: `Text`
- `name_en_1`: `Text`
- `name_fr_1`: `Text`
- `inst_identifier_1`: `Text`
- `inst_name_1`: `Text`
- `parliament_session_1`: `Text`
- `updated_at_2`: `Timestamp`
- `latest_action_dt_2`: `Date`
- `id_2`: `Int`
- `jurisdiction_id_2`: `Int`
- `jurisdiction_name_2`: `Text`
- `legal_type_id_2`: `Int`
- `name_2`: `Text`
- `name_en_2`: `Text`
- `name_fr_2`: `Text`
- `inst_identifier_2`: `Text`
- `inst_name_2`: `Text`
- `parliament_session_2`: `Text`
- `updated_at_3`: `Timestamp`
- `latest_action_dt_3`: `Date`
- `id_3`: `Int`
- `jurisdiction_id_3`: `Int`
- `jurisdiction_name_3`: `Text`
- `legal_type_id_3`: `Int`
- `name_3`: `Text`
- `name_en_3`: `Text`
- `name_fr_3`: `Text`
- `inst_identifier_3`: `Text`
- `inst_name_3`: `Text`
- `parliament_session_3`: `Text`
- `updated_at_4`: `Timestamp`
- `latest_action_dt_4`: `Date`
- `id_4`: `Int`
- `jurisdiction_id_4`: `Int`
- `jurisdiction_name_4`: `Text`
- `legal_type_id_4`: `Int`
- `name_4`: `Text`
- `name_en_4`: `Text`
- `name_fr_4`: `Text`
- `inst_identifier_4`: `Text`
- `inst_name_4`: `Text`
- `parliament_session_4`: `Text`
- `updated_at_5`: `Timestamp`
- `latest_action_dt_5`: `Date`
- `id_5`: `Int`
- `jurisdiction_id_5`: `Int`
- `jurisdiction_name_5`: `Text`
- `legal_type_id_5`: `Int`
- `name_5`: `Text`
- `name_en_5`: `Text`
- `name_fr_5`: `Text`
- `inst_identifier_5`: `Text`
- `inst_name_5`: `Text`
- `parliament_session_5`: `Text`

`legal_scraped_jurisdiction`

- `id`: `Int64`
- `name`: `Text`
- `classification`: `Text`
- `scraped_name`: `Text`
- `updated_at`: `Timestamp`
- `extra`: `{}`
- `updated_at_1`: `Timestamp`
- `id_1`: `Int`
- `name_1`: `Text`
- `classification_1`: `Text`
- `scraped_name_1`: `Text`
- `updated_at_2`: `Timestamp`
- `id_2`: `Int`
- `name_2`: `Text`
- `classification_2`: `Text`
- `scraped_name_2`: `Text`
- `updated_at_3`: `Timestamp`
- `id_3`: `Int`
- `name_3`: `Text`
- `classification_3`: `Text`
- `scraped_name_3`: `Text`
- `updated_at_4`: `Timestamp`
- `id_4`: `Int`
- `name_4`: `Text`
- `classification_4`: `Text`
- `scraped_name_4`: `Text`
- `updated_at_5`: `Timestamp`
- `id_5`: `Int`
- `name_5`: `Text`
- `classification_5`: `Text`
- `scraped_name_5`: `Text`

`legal_event`

- `id`: `Int64`
- `jurisdiction_id`: `Int64`
- `jurisdiction_name`: `Text`
- `name`: `Text`
- `start_date`: `Date`
- `end_date`: `Date`
- `classification`: `Text`
  - Enum: `"Committee Meeting"`, `"Hearing"`, `"Reading"`, `"Vote"`, `"Other"`
- `updated_at`: `Timestamp`
- `extra`: `{}`
- `updated_at_1`: `Timestamp`
- `id_1`: `Int`
- `jurisdiction_id_1`: `Int`
- `jurisdiction_name_1`: `Text`
- `name_1`: `Text`
- `start_date_1`: `Date`
- `end_date_1`: `Date`
- `classification_1`: `Text`
- `updated_at_2`: `Timestamp`
- `id_2`: `Int`
- `jurisdiction_id_2`: `Int`
- `jurisdiction_name_2`: `Text`
- `name_2`: `Text`
- `start_date_2`: `Date`
- `end_date_2`: `Date`
- `classification_2`: `Text`
- `updated_at_3`: `Timestamp`
- `id_3`: `Int`
- `jurisdiction_id_3`: `Int`
- `jurisdiction_name_3`: `Text`
- `name_3`: `Text`
- `start_date_3`: `Date`
- `end_date_3`: `Date`
- `classification_3`: `Text`
- `updated_at_4`: `Timestamp`
- `id_4`: `Int`
- `jurisdiction_id_4`: `Int`
- `jurisdiction_name_4`: `Text`
- `name_4`: `Text`
- `start_date_4`: `Date`
- `end_date_4`: `Date`
- `classification_4`: `Text`
- `updated_at_5`: `Timestamp`
- `id_5`: `Int`
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- `jurisdiction_name_5`: `Text`
- `name_5`: `Text`
- `start_date_5`: `Date`
- `end_date_5`: `Date`
- `classification_5`: `Text`

`legal_jurisdiction`

- `id`: `Int64`
- `name`: `Text`
- `classification`: `Text`
- `jurisdiction_type`: `Text`
  - Enum: `"Federal"`, `"Provincial"`, `"Municipal"`, `"International"`
- `updated_at`: `Timestamp`
- `extra`: `{}`
- `updated_at_1`: `Timestamp`
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- `name_1`: `Text`
- `classification_1`: `Text`
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- `classification_2`: `Text`
- `jurisdiction_type_2`: `Text`
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- `classification_3`: `Text`
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- `updated_at_4`: `Timestamp`
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- `jurisdiction_type_4`: `Text`
- `updated_at_5`: `Timestamp`
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- `name_5`: `Text`
- `classification_5`: `Text`
- `jurisdiction_type_5`: `Text`

`legal_person`

- `id`: `Int64`
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- `sort_name`: `Text`
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- `death_date`: `Text`
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- `extra`: `{}`
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- `updated_at_1`: `Timestamp`
- `id_1`: `Int`
- `name_1`: `Text`
- `sort_name_1`: `Text`
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- `death_date_1`: `Text`
- `image_1`: `Text`
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- `birth_date_2`: `Text`
- `death_date_2`: `Text`
- `image_2`: `Text`
- `original_jurisdiction_id_2`: `Text`
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- `death_date_3`: `Text`
- `image_3`: `Text`
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- `updated_at_4`: `Timestamp`
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- `name_4`: `Text`
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- `death_date_5`: `Text`
- `image_5`: `Text`
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`legal_vote_event`

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- `jurisdiction_id`: `Int64`
- `jurisdiction_name`: `Text`
- `legislative_session`: `Text`
- `motion_text`: `Text`
- `start_date`: `Date`
- `classification`: `[Text]`
- `result`: `Text`
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- `updated_at`: `Timestamp`
- `extra`: `{}`
- `updated_at_1`: `Timestamp`
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- `jurisdiction_id_1`: `Int`
- `jurisdiction_name_1`: `Text`
- `legislative_session_1`: `Text`
- `motion_text_1`: `Text`
- `start_date_1`: `Date`
- `classification_1`: `[Text]`
- `result_1`: `Text`
- `updated_at_2`: `Timestamp`
- `id_2`: `Int`
- `jurisdiction_id_2`: `Int`
- `jurisdiction_name_2`: `Text`
- `legislative_session_2`: `Text`
- `motion_text_2`: `Text`
- `start_date_2`: `Date`
- `classification_2`: `[Text]`
- `result_2`: `Text`
- `updated_at_3`: `Timestamp`
- `id_3`: `Int`
- `jurisdiction_id_3`: `Int`
- `jurisdiction_name_3`: `Text`
- `legislative_session_3`: `Text`
- `motion_text_3`: `Text`
- `start_date_3`: `Date`
- `classification_3`: `[Text]`
- `result_3`: `Text`
- `updated_at_4`: `Timestamp`
- `id_4`: `Int`
- `jurisdiction_id_4`: `Int`
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- `start_date_5`: `Date`
- `classification_5`: `[Text]`
- `result_5`: `Text`

`search_parameters`

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- `search_fuzzy`: `Boolean`
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- `search_offset`: `Int`
- `search_cursor`: `Text`
- `search_sort`: `Text`
  - Enum: `"relevance"`, `"id_asc"`, `"id_desc"`, `"updated_at_asc"`, `"updated_at_desc"`, `"latest_action_dt_asc"`, `"latest_action_dt_desc"`, `"start_date_asc"`, `"start_date_desc"`, `"name_asc"`, `"name_desc"`
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`search_results`

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- `search_type`: `Text`
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- `search_offset`: `Int`
- `search_limit`: `Int`
- `search_cursor`: `Text`
- `search_next_cursor`: `Text`
- `search_has_more`: `Boolean`
- `search_results`: `[{}]`

`legal`

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- `jurisdiction_id`: `Int64`
- `jurisdiction_name`: `Text`
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- `name_fr`: `Text`
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- `inst_identifier`: `Text`
- `inst_classification`: `Text`
- `inst_name`: `Text`
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- `latest_motion`: `Text`
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- `abstract`: `Text`
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- `other_dates`: `[{}]`
- `related_bills`: `[{}]`
- `sources`: `[{}]`
- `sponsors`: `[{}]`
- `votes`: `[{}]`
- `extras`: `{}`

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`legal_event`

- `id`: `Int64`
- `jurisdiction_id`: `Int64`
- `jurisdiction_name`: `Text`
- `name`: `Text`
- `start_date`: `Date`
- `end_date`: `Date`
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- `updated_at`: `Timestamp`
- `extra`: `{}`

`legal_jurisdiction`

- `id`: `Int64`
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- `classification`: `Text`
- `jurisdiction_type`: `Text`
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`legal_person`

- `id`: `Int64`
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- `sort_name`: `Text`
- `email`: `Text`
- `biography`: `Text`
- `gender`: `Text`
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- `death_date`: `Text`
- `image`: `Text`
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- `updated_at`: `Timestamp`

`legal_vote_event`

- `id`: `Int64`
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- `result`: `Text`
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- `updated_at`: `Timestamp`
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- `search_fuzzy`: `Boolean`
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- `search_cursor`: `Text`
- `search_sort`: `Text`
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`search_results`

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- `search_next_cursor`: `Text`
- `search_has_more`: `Boolean`
- `search_results`: `[{}]`

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- `jurisdiction_name`: `Text`
- `name`: `Text`
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- `end_date`: `Date`
- `updated_at`: `Timestamp`
- `extra`: `{}`

`search_parameters`

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- `search_mode`: `Text`
  - Enum: `"plain"`, `"phrase"`, `"prefix"`, `"boolean"`, `"websearch"`
- `search_lang`: `Text`
- `search_fuzzy`: `Boolean`
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- `search_offset`: `Int`
- `search_cursor`: `Text`
- `search_sort`: `Text`
  - Enum: `"relevance"`, `"id_asc"`, `"id_desc"`, `"updated_at_asc"`, `"updated_at_desc"`, `"latest_action_dt_asc"`, `"latest_action_dt_desc"`, `"start_date_asc"`, `"start_date_desc"`, `"name_asc"`, `"name_desc"`
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`search_results`

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- `search_limit`: `Int`
- `search_cursor`: `Text`
- `search_next_cursor`: `Text`
- `search_has_more`: `Boolean`
- `search_results`: `[{}]

PHENIX

Python based Hierarchical Environment for Integrated Xtallography

Automated protein-ligand structure determination with phenix.fpend_pipeline

Contents

- Overview
- Input files
- Overall workflow
- Interactive mode
- Output files
- Limitations
- Troubleshooting
- Next steps
- Other related pipelines
- Acknowledgements
- List of all available keywords

Overview

phenix.fpend_pipeline is a fully automated ligand identification, fitting, refinement, validation, visualization and curation, with optional interaction with coot. It features many, if not most, of the features and options of phenix.ligandfit, phenix.refine and phenix.fmodel, and adds some additional options and features that are unique to the fpend pipeline.

Input files

phenix.fpend_pipeline takes the same kinds of processed experimental data, a starting model for molecular replacement, and a ligand file as phenix.ligandfit, and adds a number of optional parameters which are used, for instance, in phenix.refine and phenix.fmodel. Because phenix.fpend_pipeline runs all three programs, it requires a number of input parameters.

```
phenix.fpend_pipeline data.mtz model.pdb ligand.cif
```

The data mtz file can be PHENIX or CCP4 Mtz files and should ideally contain all the parameters automatically, but one may also supply the flags in a separate file (i.e. `data.mtz.labels.txt`). This is especially recommended if you want to use a specific set of reflections for cross-validation (R free flags) or phenix.refine will create a new set.

To specify the ligand geometry, general ligand restraints options are available:

- Chemical file, such as PDB, CIF (files can include existing restraints), or SMILES: `ligand=ligand.cif`
- Ligand name: `ligand=ATP`
- The ligand already present in the PDB: if one knows the three letter code used, one may specify this `ligand=ATP,ADP`

It is recommended that one use the most detailed and explicit information about the ligand chemistry and connectivity, and specify the ligand name if it is present in the starting model. If one does not, the program will attempt to guess a suitable chemical description, but one should be aware that this may be difficult and may lead to errors. Specifying the ligand name will also allow the program to use the ligand in the starting model as a template for the ligand fit, which may be helpful if the ligand is not well supported by the density. Specifying the chemical file refinement with the `ref.ligand` keyword. This should also specify `ref.ligand.fix` to prevent phenix.refine from modifying the ligand geometry.

Finally, if the data or the ligand directory and their pipe can be unambiguously determined, one may supply the directory name instead of the file specifying the ligand:

```
phenix.fpend_pipeline data/ ligand/ model.pdb
```

Program workflow

Data preparation: The program begins by inspecting the experimental data and converting it to amplitudes with phenix.reflection_preparation if necessary. It then runs phenix.xtriage to check for twinning and other issues that may cause problems for refinement and downstream analysis. Twinning, if detected, will be by default treated in the refinement and model building steps, but not in the initial molecular replacement step, because the number of reflections is too low.

Molecular replacement: The MR step is run on the input ligand-deficient PDB model using phenix.ligandfit with the `ligand.remove` option. This step is optional, but it is highly recommended because it generally results in a more-interesting, but in some cases it may lead to incorrect geometry. For homologous models, we recommend using phenix.sculptor to remove side chains and phenix.chainsaw to remove loops. Alternatively, one may specify `ref.ignore_if_no_ligand=True` in the PDB. If one knows the three letter code used, one may specify this `ligand=ATP,ADP`.

Model preparation: For each input model, a series of cleanup steps is run to remove specific details such as non-standard residues, alternate conformations, and ligands. The cleaned models are then used for refinement, and the original versions kept unaltered. CRYs and the ordered solvent molecules, and this is suitable as a starting model for refinement.

Model placement: Two options are available, rigid-body refinement or molecular replacement:

- **Molecular replacement**: This uses the default MR step in phenix. Work includes rigid-body and real-space refinement, and optional side chain rotamer fitting. Ligand placement and fitting are determined automatically by Xtriage (`ligand.fit`), but since this will unnecessarily guess the two cases, one may specify `ligand.fit=True` or `ligand.fit=False` to force the program to perform ligand fitting or not. Ligand placement is based on the density and on the ligand's centroid. Alternatively, one may specify a specific ligand location by specifying `ligand.xyz=x,y,z`. Ligand fitting is performed using phenix.ligandfit, and the ligand is added to the model before refinement.
- **Rigid-body refinement**: If this mode is already close enough to the target structure, rigid-body refinement may be sufficient.

Currently MR is by default, but this will be changed in the future. If you are confident that the model can be placed by rigid-body refinement, specify `ligand.fit=False`. If you are confident that the ligand is present, specify `ligand.fit=True` or specify the ligand location with `ligand.xyz=x,y,z`. Alternatively, one may specify `ligand.fit=auto` to prevent phenix.ligandfit from fitting the ligand.

Finally, if the data or the ligand directory and their pipe can be unambiguously determined, one may supply directory name instead of the file specifying the ligand:

```
phenix.fpend_pipeline data/ ligand/ model.pdb
```

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- **Molecular replacement**: This uses the default MR step in phenix. Work includes rigid-body and real-space refinement, and optional side chain rotamer fitting. Ligand placement and fitting are determined automatically by Xtriage (`ligand.fit`), but since this will unnecessarily guess the two cases, one may specify `ligand.fit=True` or `ligand.fit=False` to force the program to perform ligand fitting or not. Ligand placement is based on the density and on the ligand's centroid. Alternatively, one may specify a specific ligand location by specifying `ligand.xyz=x,y,z`. Ligand fitting is performed using phenix.ligandfit, and the ligand is added to the model before refinement.
- **Rigid-body refinement**: If this mode is already close enough to the target structure, rigid-body refinement may be sufficient.

Currently MR is by default, but this will be changed in the future. If you are confident that the model can be placed by rigid-body refinement, specify `ligand.fit=False`. If you are confident that the ligand is present, specify `ligand.fit=True` or specify the ligand location with `ligand.xyz=x,y,z`. Alternatively, one may specify `ligand.fit=auto` to prevent phenix.ligandfit from fitting the ligand.

In summary, in MR mode, you may specify multiple models as input, the best model will be selected either by default or based on the keywords. The ligand will be placed by phenix.ligandfit, and refinement will be performed with phenix.refine.

Initial refinement: The first step of refinement is phenix.refine. PDB files are preferred, and the default output features conservative reasonable restraints, default refinement strategy, default refinement weight, and default output. Ordinarily, one would want to use the default output, but in some cases, one may want to use the output of phenix.ligandfit or phenix.refine as input for the next step. Alternatively, one may specify `ref.ignore_ligandfit=True` or `ref.ignore_refine=True` to ignore the output of phenix.ligandfit or phenix.refine, respectively. Ordinarily, the structure is expected to be the same as the starting model, but if one specifies `ref.ignore_ligandfit=True`, the starting model will be used instead of the output of phenix.ligandfit. Finally, if one specifies `ref.ignore_ligandfit=False`, the output of phenix.ligandfit will be used, but the output of phenix.refine will be ignored. Other options are available, such as `ref.ignore_ligand=True` to remove the ligand from the structure before refinement, and `ref.ignore_ligand.fit=True` to force ligand fitting and refinement to be performed in the same step.

Refinement: Refinement is by default performed with phenix.refine, but one may also use phenix.fmodel. Refinement is performed with default parameters, but one may specify `ref.refine.strategy=rigid_body,tls,xyz,adp` to specify the refinement strategy, `ref.refine.weight=1.0` to specify the refinement weight, and `ref.refine.output=pdb,cif` to specify the output files. Refinement is performed for a specified number of cycles, by default 5, but one may specify `ref.refine.cycles=10` to specify the number of cycles. Finally, one may specify `ref.refine.ignore_ligand=True` to remove the ligand from the structure before refinement.

Ligand placement: Currently only LigandFit is supported, although additional options will be available in the future. Ordinarily, one would want to use the default output, but in some cases, one may want to use the output of phenix.ligandfit as input for the next step. Alternatively, one may specify `ligand.ignore_ligandfit=True` to ignore the output. Most ligand refinements will be performed by Ligandfit after refinement is ended, or after refinement has ended, but one may specify `ligand.fit=True` to force ligand fitting and refinement to be performed in the same step.

Ordinarily, one would want to use the default output, but in some cases, one may want to use the output of phenix.ligandfit as input for the next step. Alternatively, one may specify `ligand.ignore_ligandfit=True` to ignore the output. Most ligand refinements will be performed by Ligandfit after refinement is ended, or after refinement has ended, but one may specify `

Other notes about use

Security notes Not all of the contents in search editing the market, the default protocol is very robust but not especially fast, and they be correspondently intended for data codes. You can send to a Tokeat protocol to the Tokeat protocol, and it will be sent to the Tokeat protocol, and it will be sent to the Tokeat protocol.

Warnings

Warning about Tokeat can be called out of the Tokeat infrastructure Tokeat, and the use Tokeat protocol, and Tokeat protocol, and use Tokeat as high reputation, however, it has the side effect of making information available to the Tokeat infrastructure, and Tokeat protocol, and Tokeat.

Matching criterion Indicates included by a process step Duration of the process step, or missing in the input Duration, may specially be replaced after signal presented by specifying unsuccessful.

Tokeat protocol Tokeat protocol, and Tokeat protocol, and Tokeat protocol, and

Automated ligand fitting with LigandFit

Contents

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- Specifying which columns of data to use from input data files
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- **Examples**
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- Keywords for LigandFit
- **See Also**
- Tutorials on the LigandFit Wizard
- **Acknowledgments**
- **Last updated: October 2, 2009**

Author(s)

- Tom Terwilliger, Tom Terwilliger
- PHENIX Software Development Team
- Ralf W. Grosse-Kunstleve, Ralf W. Grosse-Kunstleve

Purpose

Purpose of the LigandFit Wizard

The LigandFit Wizard carries out fitting of flexible ligands to electron density maps.

Usage

The LigandFit Wizard can be run from the PHENIX GUI, from the command line, and from parameters files. All examples here are based on the command line. The command line version of the LigandFit Wizard is the PHENIX module phenix.ligandfit. Details of how to run it follow. The command line version will be described here.

How the LigandFit Wizard works

The LigandFit Wizard is a wizard that provides a simplified user interface allowing the user to identify a ligand, preparing a ligand model, and fitting it into electron density. It operates from the user's point of view in the following way: the user provides a map and a model, and the LigandFit Wizard finds the ligand in the combined map.

The LigandFit Wizard first takes the coordinates and then uses RESOLVE to carry out the fitting of the ligand into the electron density map. This step may be run in parallel. It fits in rigid body pieces which, first, can vary from LigandFit version to LigandFit version, and, second, can be fitted in a fixed order (standard mode) or with groups fitted in random order (random mode). The pieces are fitted into the electron density map and the best fit is selected. The best fit is defined as the fit with the highest correlation between the electron density and a model calculated from the ligand. In the case of a flexible ligand, the best fit is the ligand with correlation to the electron density map closest to the map value of the ligand.

The ligand fitting is done by RESOLVE in a three-stage process. First, the ligand conformer library of density is fitted into the electron density map using a rigid body search. The best fit is then used as a starting point for a second search in which the ligand is broken into two rigid pieces which are fitted into the electron density map. The best fit is then used as a starting point for a third search in which the ligand is broken into three rigid pieces which are fitted into the electron density map. The best fit is then used as a starting point for a final refinement of the ligand. In the case of a flexible ligand, the best fit is the ligand with correlation to the electron density map closest to the map value of the ligand. In the case of a rigid ligand, the best fitting placement is also out of the ligand.

The LigandFit Wizard then takes the best fit ligand and prepares a model for refinement. This step includes the Polishit module of Ligandfit and the R-to-S-to-Ligand-to-Polishit-to-Ligand-to-Polishit-to-Ligand-to-Polishit

```
[Tipsy] [Lucy] [Lucy]
```

Tipsy and Lucy are two contrast sets which have group of species (so that tipsyRich can identify the position and correlation of species and lucyRich can do the same for Lucy).

- the RICH from the model and the first tipsyRich tipsy to guess the positions of RICH related tipsyRich
- the RICH from the model and the first lucyRich lucy to guess the positions of RICH related lucyRich

```
[Tipsy] [Lucy] [Lucy]
```

R-free flags and test set

Both Tipsy and Lucy need a test set to calculate the value of the test set that is not in the Rfree flags. Normally Rfree will be used as the test set but if Lucy is run in the map mode, the Rfree parameters is used for Fourier transform and the test set is the set that is not in the Rfree flags. Tipsy will use the test set to calculate the R-free and the R-free flag value is recorded into mtzfile output of Lucy and tipsy will use it to check you are satisfy that with the R-free flags.

Using LibraryFit with an mtz map as input

You can run Tipsy fitting using an mtz or ccp4 map file as input instead of using map coefficients. If you specify a map file, Tipsy will calculate the map coefficients using the phases from the model and use that map to compare to the map coefficients in the reflection file. Tipsy will use the map coefficients in the reflection file to calculate the R-factor and R-free.

If one supply a map that has an origin offset (a lesser map), then the map will be recentered to map coefficients and the model will be shifted to the new origin. Tipsy will write out the shifted model and the new map.

If your map has an origin offset that is qualified by an unknown map, the external map is recentered to the origin of the model. Tipsy will write out the shifted model. Note that not all Mapman programs can properly display maps with non-zero origins.

Possible Problems

In some cases Ipsyn fitting results in an incompatible ligand (some atoms are missing). Here is a procedure you can use to correct the problem:

- find the fitting coordinates in the file in the form called "Rejected Ligand" (use the search function in your text editor to find the word "Rejected" in the file ending with .pdb)
- Take your official ".cif" library (ligand.cif) and "prune" (remove) atoms from the library to make a new library that matches the rejected ligand. (Note: the atom names in the library and in the rejected ligand must be the same for this to work)
- Run libraryfit with the new library and the rejected ligand as input.

Specific limitations and problems

- The ligand is not expected to be more than about 4 planes.
- Tipsy will not work with ligands that have covalent bonds to protein residues, which are automatically removed in the position where the ligand is to be built. (If one has covalence where other bond radii suggest to be positive - Tipsy will not work. Tipsy will not work with ligands that have covalent bonds to protein residues.
- If a ligand is too large and does not fit into the binding site, Tipsy will not work. (Tipsy will work with ligands that are bigger than the binding site, but it will not work if the ligand does not fit into the binding site.)
- If you want to build your ligand manually (or if Ipsyn works only partially), then use the libraryfit program to create a library for your ligand. Then use the Ipsyn program with the new library and the rejected ligand as input.
- Libraryfit generates Coordinate Lookup, so if you specify a reactive with ligand name, you only find reactive number 1.
- The use of the assumption: Left is the BOUNDREGION position of the ligand(s) search is limited to the BOUNDREGION. Tipsy will not work if the ligand is not in the BOUNDREGION. Tipsy will not work if the ligand is not within 1 angstrom of the BOUNDREGION. Tipsy will not work if the ligand is more than 1 angstrom from the BOUNDREGION. Tipsy will not work if the ligand is not in the BOUNDREGION. Tipsy will not work if the ligand is not within 1 angstrom of

Phenix *Python based Hierarchical Environment for Integrated Xtallography*

Using the LigandFit GUI

Contents:

- Overview
- Configuration
- Running the program
- Output
- Tutorials

Overview

LigandFit is one of the four PHENIX "wizards" for automated structure determination. It performs flexible ligand fitting into difference maps using RESOLVE. Followed by optional rest-space refinement, its selections, the resulting models and maps are fed into the next step in the automated structure determination process, which is most-likely an automated model building procedure, for example using the AutoBuild wizard. Alternatively, the LigandFit wizard can be used as a stand-alone tool for ligand fitting, for example in order to see how well a particular ligand fits into the electron density, or to compare two different ligands.

Note that wizards will be omitted when placing the ligand. However, if you are using pre-calculated map coefficients, you may want to use the wizard instead of the command line version, because the wizard allows you to specify atom selections using the ligand identifiers, will prevent a mistyped phenomenon, or show selections of the ligand in the molecular graphics.

Configuration

The top of the LigandFit wizard contains a field for setting input files, which can be dragged and dropped from the Phenix File Manager or by browsing for files using the "+" button.

To run, you will need the following input files:

- A PDB file containing the ligand free model. (It is okay for this to contain polymeric molecules, waters, and other ligands, but it should not contain the ligand.)
- An MTZ file containing phases and/or map coefficients (FOBS/FC or pre-calculated difference map coefficients, for example from Refine).
- A file describing your ligand. This should be either a PDB file containing a single residue, or a chemical description (.cif/.pdb/.mol/.sdf/.mol2/.mol3/.smi/.smiles/.inchi/.inch/.inchi-key/.inch-key/.smarts/.smarts-pos/.smiles-pos/.smiles-name/.smiles-pos-name/.smarts-name/.smarts-pos-name/.smiles-name-pos/.smarts-name-pos/.smiles/.smarts/.smiles-name-pos/.smarts-name-pos/.smiles-name/.smarts-name

As a general rule, a correlation coefficient (CC) above 0.7 is considered a good fit. CC values less valid usually indicate that the region is not about correctly identified or not sized. Note that CC values are sensitive to the resolution of the map, so it is important to use the same resolution when comparing different models. The CCP4MG tool also unable to show the ligand correctly, there are several recommendations for troubleshooting:

If you do not see the ligand in the map, there are several possible reasons:

- Ligand was added to the map after the chemical formula was set to the ligand. Check in the GUI if you still need to choose these before ligandFit run for the ligand chain. The LigandFit wizard automatically sets the chemical formula for the ligand chain. **Check the ligand chain in the Molecule Tree and set the chemical formula if it is not set. Then, recalculate the map. Recalculating the ligand chain will not be enough as ligand is "hidden" if not set.**
- Ligand is too far from the protein. Check the distance between the ligand and the protein. Ligand should be within 5 Å from the protein. Check the ligand chain in the Molecule Tree and recenter (ctrl + L) the view if nothing shows up. Unselect all and then the ligand chain.
- Ligand is too small. Check the ligand size.
- Ligand is out of the difference electron density map. Check if your map density for the ligand is positive. Ligand should be in the difference electron density map. Check if your map is weighted with DFc (map that should normally show the placement of your ligand).
- Ligand is in the difference electron density map but LigandFit cannot place it. Check if your density is too noisy. Ligand should be in the difference electron density map. Check if your density is too noisy. Check the ligand chain in the Molecule Tree and recenter (ctrl + L) the view if nothing shows up. Unselect all and then the ligand chain.

References

- **Ligand identification using electron density map correlations.** T.C. Terwilliger, P.D. Adams, R.W. Read, D.W. Adams, P.H. Zwart, R.J. Gildea, L.W. Hung, R.O. Moriarty, and T.C. Terwilliger. doi:10.1107/S0907444909039764 IUCr (2009)

Optimizing a map with local_anisc_sharpen (deprecated, use MapSharpening)

Author(s)

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Purpose

This module local_anisc_sharpen is a tool for optimizing a map by applying a local, anisotropic, resolution-dependent sharpening.

How local_anisc_sharpen works:

Local anisotropic sharpening can be carried out locally, as the volume surrounding, or on a map as a whole.

The basis for sharpening is an analysis of the resolution-dependent fall off of anisotropies of Fourier coefficients. This fall off is fitted to a function of resolution and direction in reciprocal space. The function is used to sharpen or blur a density-modified map.

When applied to a map, it is not clear what the correct sharpening is. The optimal sharpening depends on the resolution of the map, the quality of the map, and the intended use of the map. The optimal sharpening can be specified by a single parameter, the sharpening factor. The sharpening factor is the factor by which the fall off of the map is to be multiplied. The sharpening factor can be estimated by comparing the fall off of the map to the fall off of a map that has been sharpened by a factor of 1.0.

To specify the optimal anisotropic sharpening of a map based on the information in two half-maps, two analyses are carried out. The first analysis is carried out on the two half-maps. The second analysis is carried out on the difference map. The first analysis and the second analysis are combined to yield the optimal sharpening. The combination is carried out by adding the two analyses and then fitting the resulting sum to a function of resolution and direction in reciprocal space. The function is used to sharpen the map.

The second is an analysis of the correlation between Fourier coefficients for the two half-maps. This is also done as a function of resolution and direction in reciprocal space. This analysis shows the anisotropy of the errors in the map.

For purposes of this analysis, the optimal map is the one that has the maximum expected correlation to an unknown map that has the same fall off of Fourier coefficients as the two half-maps and which is modified by a factor of the square root of one minus the square of error.

For a map with no error, the optimal sharpening factor is 1.0. For a map with some error, the optimal sharpening factor is less than one. The amount of sharpening depends on the resolution of the map and the amount of error in the map. The optimal sharpening factor can be estimated by comparing the fall off of the map to the fall off of a map that has been sharpened by a factor of 1.0.

For a map with errors, the map coefficients obtained from the previous step are modified by a local scale factor, which is the square root of one minus the square of the local error. The local error is estimated by the correlation of the two half-maps. The local scale factor is applied to the Fourier coefficients and added to the expected coefficients and in order to be sufficient. This scale factor will be a function of resolution and direction.

Examples

You can use local_anisc_sharpen with either two half-maps or a map and a model.

Standard run of local_anisc_sharpen with two half-maps:

```
phenix.local_anisc_sharpen map_1.ccp4 map_2.ccp4 seq.dat
phenix.local_anisc_sharpen half_map_1.ccp4 half_map_2.ccp4 resolution=3.0
```

If you wish, you can specify a minimal resolution. The sequence file is to let the program figure out the volume of the map and the number of copies.

To run local_anisc_sharpen with a map and model, you can use:

```
phenix.local_anisc_sharpen map.ccp4 model.pdb resolution=3.0 seq_file=seq.fasta
```

The resolution is again optional.

You can specify whether anisotropy or local sharpening are to be applied:

```
phenix.local_anisc_sharpen
  map_1.ccp4 map_2.ccp4 seq.dat
  anisotropy=true local_sharpening=false
```

Output

local_anisc_sharpen will provide a summary of the analysis of your map if you leave anisotropy_sharpen=true. Here are some of the values that are calculated for a half-map, with anisotropy:

```
MPEG Ext Group Water Level Changes (Version 1.0)
  Ext Group Header Block (GHB) Structure
  ------------------------------------------------------------
  ------------------------------------------------------------
  This section is valid for the water level data files.
  The GHB is a 512 byte block of data, which follows the
  Main Header Block (MHB) and precedes the first group
  header.
  The GHB contains the Extended Group Water Level Data
  Header Block (EGWLDHB).

  The EGWLDHB contains a variable-length array of
  Water Level Data Descriptor Blocks (WLDDB) which
  describe the water level data in the data blocks
  following the group header.

  Unlimited Accuracy Scl/Off of the data values is then
  applied to the data to get the final data values.
  (A.Wl, A.Wl, A.Wl, A.Wl, A.Wl, A.Wl, A.Wl, A.Wl)

  This is the Scl/Off of the data after removal of the effect of tides.
  This is the Scl/Off of the data after removal of the effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise. This is the recommended Scl/Off to use for most
  applications.
  (A.Wl, A.Wl, A.Wl, A.Wl, A.Wl, A.Wl, A.Wl, A.Wl)

  Unlimited Accuracy Scl/Off of the data values is then
  applied to the data to get the final data values.
  (B.Wl, B.Wl, B.Wl, B.Wl, B.Wl, B.Wl, B.Wl, B.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (B.Wl, B.Wl, B.Wl, B.Wl, B.Wl, B.Wl, B.Wl, B.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (C.Wl, C.Wl, C.Wl, C.Wl, C.Wl, C.Wl, C.Wl, C.Wl)

  Unlimited Accuracy Scl/Off of the data values is then
  applied to the data to get the final data values.
  (D.Wl, D.Wl, D.Wl, D.Wl, D.Wl, D.Wl, D.Wl, D.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (E.Wl, E.Wl, E.Wl, E.Wl, E.Wl, E.Wl, E.Wl, E.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (F.Wl, F.Wl, F.Wl, F.Wl, F.Wl, F.Wl, F.Wl, F.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (G.Wl, G.Wl, G.Wl, G.Wl, G.Wl, G.Wl, G.Wl, G.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (H.Wl, H.Wl, H.Wl, H.Wl, H.Wl, H.Wl, H.Wl, H.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (I.Wl, I.Wl, I.Wl, I.Wl, I.Wl, I.Wl, I.Wl, I.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (J.Wl, J.Wl, J.Wl, J.Wl, J.Wl, J.Wl, J.Wl, J.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (K.Wl, K.Wl, K.Wl, K.Wl, K.Wl, K.Wl, K.Wl, K.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (L.Wl, L.Wl, L.Wl, L.Wl, L.Wl, L.Wl, L.Wl, L.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (M.Wl, M.Wl, M.Wl, M.Wl, M.Wl, M.Wl, M.Wl, M.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (N.Wl, N.Wl, N.Wl, N.Wl, N.Wl, N.Wl, N.Wl, N.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (O.Wl, O.Wl, O.Wl, O.Wl, O.Wl, O.Wl, O.Wl, O.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (P.Wl, P.Wl, P.Wl, P.Wl, P.Wl, P.Wl, P.Wl, P.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (Q.Wl, Q.Wl, Q.Wl, Q.Wl, Q.Wl, Q.Wl, Q.Wl, Q.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (R.Wl, R.Wl, R.Wl, R.Wl, R.Wl, R.Wl, R.Wl, R.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (S.Wl, S.Wl, S.Wl, S.Wl, S.Wl, S.Wl, S.Wl, S.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (T.Wl, T.Wl, T.Wl, T.Wl, T.Wl, T.Wl, T.Wl, T.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (U.Wl, U.Wl, U.Wl, U.Wl, U.Wl, U.Wl, U.Wl, U.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (V.Wl, V.Wl, V.Wl, V.Wl, V.Wl, V.Wl, V.Wl, V.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (W.Wl, W.Wl, W.Wl, W.Wl, W.Wl, W.Wl, W.Wl, W.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (X.Wl, X.Wl, X.Wl, X.Wl, X.Wl, X.Wl, X.Wl, X.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (Y.Wl, Y.Wl, Y.Wl, Y.Wl, Y.Wl, Y.Wl, Y.Wl, Y.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (Z.Wl, Z.Wl, Z.Wl, Z.Wl, Z.Wl, Z.Wl, Z.Wl, Z.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AA.Wl, AA.Wl, AA.Wl, AA.Wl, AA.Wl, AA.Wl, AA.Wl, AA.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AB.Wl, AB.Wl, AB.Wl, AB.Wl, AB.Wl, AB.Wl, AB.Wl, AB.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AC.Wl, AC.Wl, AC.Wl, AC.Wl, AC.Wl, AC.Wl, AC.Wl, AC.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AD.Wl, AD.Wl, AD.Wl, AD.Wl, AD.Wl, AD.Wl, AD.Wl, AD.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AE.Wl, AE.Wl, AE.Wl, AE.Wl, AE.Wl, AE.Wl, AE.Wl, AE.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AF.Wl, AF.Wl, AF.Wl, AF.Wl, AF.Wl, AF.Wl, AF.Wl, AF.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AG.Wl, AG.Wl, AG.Wl, AG.Wl, AG.Wl, AG.Wl, AG.Wl, AG.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AH.Wl, AH.Wl, AH.Wl, AH.Wl, AH.Wl, AH.Wl, AH.Wl, AH.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AI.Wl, AI.Wl, AI.Wl, AI.Wl, AI.Wl, AI.Wl, AI.Wl, AI.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AJ.Wl, AJ.Wl, AJ.Wl, AJ.Wl, AJ.Wl, AJ.Wl, AJ.Wl, AJ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AK.Wl, AK.Wl, AK.Wl, AK.Wl, AK.Wl, AK.Wl, AK.Wl, AK.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AL.Wl, AL.Wl, AL.Wl, AL.Wl, AL.Wl, AL.Wl, AL.Wl, AL.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AM.Wl, AM.Wl, AM.Wl, AM.Wl, AM.Wl, AM.Wl, AM.Wl, AM.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AN.Wl, AN.Wl, AN.Wl, AN.Wl, AN.Wl, AN.Wl, AN.Wl, AN.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AO.Wl, AO.Wl, AO.Wl, AO.Wl, AO.Wl, AO.Wl, AO.Wl, AO.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AP.Wl, AP.Wl, AP.Wl, AP.Wl, AP.Wl, AP.Wl, AP.Wl, AP.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AQ.Wl, AQ.Wl, AQ.Wl, AQ.Wl, AQ.Wl, AQ.Wl, AQ.Wl, AQ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AR.Wl, AR.Wl, AR.Wl, AR.Wl, AR.Wl, AR.Wl, AR.Wl, AR.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AS.Wl, AS.Wl, AS.Wl, AS.Wl, AS.Wl, AS.Wl, AS.Wl, AS.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AT.Wl, AT.Wl, AT.Wl, AT.Wl, AT.Wl, AT.Wl, AT.Wl, AT.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AU.Wl, AU.Wl, AU.Wl, AU.Wl, AU.Wl, AU.Wl, AU.Wl, AU.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AV.Wl, AV.Wl, AV.Wl, AV.Wl, AV.Wl, AV.Wl, AV.Wl, AV.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AW.Wl, AW.Wl, AW.Wl, AW.Wl, AW.Wl, AW.Wl, AW.Wl, AW.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AX.Wl, AX.Wl, AX.Wl, AX.Wl, AX.Wl, AX.Wl, AX.Wl, AX.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AY.Wl, AY.Wl, AY.Wl, AY.Wl, AY.Wl, AY.Wl, AY.Wl, AY.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (AZ.Wl, AZ.Wl, AZ.Wl, AZ.Wl, AZ.Wl, AZ.Wl, AZ.Wl, AZ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BA.Wl, BA.Wl, BA.Wl, BA.Wl, BA.Wl, BA.Wl, BA.Wl, BA.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BB.Wl, BB.Wl, BB.Wl, BB.Wl, BB.Wl, BB.Wl, BB.Wl, BB.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BC.Wl, BC.Wl, BC.Wl, BC.Wl, BC.Wl, BC.Wl, BC.Wl, BC.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BD.Wl, BD.Wl, BD.Wl, BD.Wl, BD.Wl, BD.Wl, BD.Wl, BD.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BE.Wl, BE.Wl, BE.Wl, BE.Wl, BE.Wl, BE.Wl, BE.Wl, BE.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BF.Wl, BF.Wl, BF.Wl, BF.Wl, BF.Wl, BF.Wl, BF.Wl, BF.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BG.Wl, BG.Wl, BG.Wl, BG.Wl, BG.Wl, BG.Wl, BG.Wl, BG.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BH.Wl, BH.Wl, BH.Wl, BH.Wl, BH.Wl, BH.Wl, BH.Wl, BH.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BI.Wl, BI.Wl, BI.Wl, BI.Wl, BI.Wl, BI.Wl, BI.Wl, BI.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BJ.Wl, BJ.Wl, BJ.Wl, BJ.Wl, BJ.Wl, BJ.Wl, BJ.Wl, BJ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BK.Wl, BK.Wl, BK.Wl, BK.Wl, BK.Wl, BK.Wl, BK.Wl, BK.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BL.Wl, BL.Wl, BL.Wl, BL.Wl, BL.Wl, BL.Wl, BL.Wl, BL.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BM.Wl, BM.Wl, BM.Wl, BM.Wl, BM.Wl, BM.Wl, BM.Wl, BM.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BN.Wl, BN.Wl, BN.Wl, BN.Wl, BN.Wl, BN.Wl, BN.Wl, BN.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BO.Wl, BO.Wl, BO.Wl, BO.Wl, BO.Wl, BO.Wl, BO.Wl, BO.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BP.Wl, BP.Wl, BP.Wl, BP.Wl, BP.Wl, BP.Wl, BP.Wl, BP.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BQ.Wl, BQ.Wl, BQ.Wl, BQ.Wl, BQ.Wl, BQ.Wl, BQ.Wl, BQ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BR.Wl, BR.Wl, BR.Wl, BR.Wl, BR.Wl, BR.Wl, BR.Wl, BR.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BS.Wl, BS.Wl, BS.Wl, BS.Wl, BS.Wl, BS.Wl, BS.Wl, BS.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BT.Wl, BT.Wl, BT.Wl, BT.Wl, BT.Wl, BT.Wl, BT.Wl, BT.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BU.Wl, BU.Wl, BU.Wl, BU.Wl, BU.Wl, BU.Wl, BU.Wl, BU.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BV.Wl, BV.Wl, BV.Wl, BV.Wl, BV.Wl, BV.Wl, BV.Wl, BV.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BW.Wl, BW.Wl, BW.Wl, BW.Wl, BW.Wl, BW.Wl, BW.Wl, BW.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BX.Wl, BX.Wl, BX.Wl, BX.Wl, BX.Wl, BX.Wl, BX.Wl, BX.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BY.Wl, BY.Wl, BY.Wl, BY.Wl, BY.Wl, BY.Wl, BY.Wl, BY.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (BZ.Wl, BZ.Wl, BZ.Wl, BZ.Wl, BZ.Wl, BZ.Wl, BZ.Wl, BZ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CA.Wl, CA.Wl, CA.Wl, CA.Wl, CA.Wl, CA.Wl, CA.Wl, CA.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CB.Wl, CB.Wl, CB.Wl, CB.Wl, CB.Wl, CB.Wl, CB.Wl, CB.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CC.Wl, CC.Wl, CC.Wl, CC.Wl, CC.Wl, CC.Wl, CC.Wl, CC.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CD.Wl, CD.Wl, CD.Wl, CD.Wl, CD.Wl, CD.Wl, CD.Wl, CD.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CE.Wl, CE.Wl, CE.Wl, CE.Wl, CE.Wl, CE.Wl, CE.Wl, CE.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CF.Wl, CF.Wl, CF.Wl, CF.Wl, CF.Wl, CF.Wl, CF.Wl, CF.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CG.Wl, CG.Wl, CG.Wl, CG.Wl, CG.Wl, CG.Wl, CG.Wl, CG.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CH.Wl, CH.Wl, CH.Wl, CH.Wl, CH.Wl, CH.Wl, CH.Wl, CH.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CI.Wl, CI.Wl, CI.Wl, CI.Wl, CI.Wl, CI.Wl, CI.Wl, CI.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CJ.Wl, CJ.Wl, CJ.Wl, CJ.Wl, CJ.Wl, CJ.Wl, CJ.Wl, CJ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CK.Wl, CK.Wl, CK.Wl, CK.Wl, CK.Wl, CK.Wl, CK.Wl, CK.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CL.Wl, CL.Wl, CL.Wl, CL.Wl, CL.Wl, CL.Wl, CL.Wl, CL.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CM.Wl, CM.Wl, CM.Wl, CM.Wl, CM.Wl, CM.Wl, CM.Wl, CM.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CN.Wl, CN.Wl, CN.Wl, CN.Wl, CN.Wl, CN.Wl, CN.Wl, CN.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CO.Wl, CO.Wl, CO.Wl, CO.Wl, CO.Wl, CO.Wl, CO.Wl, CO.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CP.Wl, CP.Wl, CP.Wl, CP.Wl, CP.Wl, CP.Wl, CP.Wl, CP.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CQ.Wl, CQ.Wl, CQ.Wl, CQ.Wl, CQ.Wl, CQ.Wl, CQ.Wl, CQ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CR.Wl, CR.Wl, CR.Wl, CR.Wl, CR.Wl, CR.Wl, CR.Wl, CR.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CS.Wl, CS.Wl, CS.Wl, CS.Wl, CS.Wl, CS.Wl, CS.Wl, CS.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CT.Wl, CT.Wl, CT.Wl, CT.Wl, CT.Wl, CT.Wl, CT.Wl, CT.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CU.Wl, CU.Wl, CU.Wl, CU.Wl, CU.Wl, CU.Wl, CU.Wl, CU.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CV.Wl, CV.Wl, CV.Wl, CV.Wl, CV.Wl, CV.Wl, CV.Wl, CV.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CW.Wl, CW.Wl, CW.Wl, CW.Wl, CW.Wl, CW.Wl, CW.Wl, CW.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CX.Wl, CX.Wl, CX.Wl, CX.Wl, CX.Wl, CX.Wl, CX.Wl, CX.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CY.Wl, CY.Wl, CY.Wl, CY.Wl, CY.Wl, CY.Wl, CY.Wl, CY.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (CZ.Wl, CZ.Wl, CZ.Wl, CZ.Wl, CZ.Wl, CZ.Wl, CZ.Wl, CZ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DA.Wl, DA.Wl, DA.Wl, DA.Wl, DA.Wl, DA.Wl, DA.Wl, DA.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DB.Wl, DB.Wl, DB.Wl, DB.Wl, DB.Wl, DB.Wl, DB.Wl, DB.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DC.Wl, DC.Wl, DC.Wl, DC.Wl, DC.Wl, DC.Wl, DC.Wl, DC.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DD.Wl, DD.Wl, DD.Wl, DD.Wl, DD.Wl, DD.Wl, DD.Wl, DD.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DE.Wl, DE.Wl, DE.Wl, DE.Wl, DE.Wl, DE.Wl, DE.Wl, DE.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DF.Wl, DF.Wl, DF.Wl, DF.Wl, DF.Wl, DF.Wl, DF.Wl, DF.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DG.Wl, DG.Wl, DG.Wl, DG.Wl, DG.Wl, DG.Wl, DG.Wl, DG.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DH.Wl, DH.Wl, DH.Wl, DH.Wl, DH.Wl, DH.Wl, DH.Wl, DH.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DI.Wl, DI.Wl, DI.Wl, DI.Wl, DI.Wl, DI.Wl, DI.Wl, DI.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DJ.Wl, DJ.Wl, DJ.Wl, DJ.Wl, DJ.Wl, DJ.Wl, DJ.Wl, DJ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DK.Wl, DK.Wl, DK.Wl, DK.Wl, DK.Wl, DK.Wl, DK.Wl, DK.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DL.Wl, DL.Wl, DL.Wl, DL.Wl, DL.Wl, DL.Wl, DL.Wl, DL.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DM.Wl, DM.Wl, DM.Wl, DM.Wl, DM.Wl, DM.Wl, DM.Wl, DM.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DN.Wl, DN.Wl, DN.Wl, DN.Wl, DN.Wl, DN.Wl, DN.Wl, DN.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DO.Wl, DO.Wl, DO.Wl, DO.Wl, DO.Wl, DO.Wl, DO.Wl, DO.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DP.Wl, DP.Wl, DP.Wl, DP.Wl, DP.Wl, DP.Wl, DP.Wl, DP.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DQ.Wl, DQ.Wl, DQ.Wl, DQ.Wl, DQ.Wl, DQ.Wl, DQ.Wl, DQ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DR.Wl, DR.Wl, DR.Wl, DR.Wl, DR.Wl, DR.Wl, DR.Wl, DR.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DS.Wl, DS.Wl, DS.Wl, DS.Wl, DS.Wl, DS.Wl, DS.Wl, DS.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DT.Wl, DT.Wl, DT.Wl, DT.Wl, DT.Wl, DT.Wl, DT.Wl, DT.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DU.Wl, DU.Wl, DU.Wl, DU.Wl, DU.Wl, DU.Wl, DU.Wl, DU.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DV.Wl, DV.Wl, DV.Wl, DV.Wl, DV.Wl, DV.Wl, DV.Wl, DV.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DW.Wl, DW.Wl, DW.Wl, DW.Wl, DW.Wl, DW.Wl, DW.Wl, DW.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DX.Wl, DX.Wl, DX.Wl, DX.Wl, DX.Wl, DX.Wl, DX.Wl, DX.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DY.Wl, DY.Wl, DY.Wl, DY.Wl, DY.Wl, DY.Wl, DY.Wl, DY.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (DZ.Wl, DZ.Wl, DZ.Wl, DZ.Wl, DZ.Wl, DZ.Wl, DZ.Wl, DZ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EA.Wl, EA.Wl, EA.Wl, EA.Wl, EA.Wl, EA.Wl, EA.Wl, EA.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EB.Wl, EB.Wl, EB.Wl, EB.Wl, EB.Wl, EB.Wl, EB.Wl, EB.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EC.Wl, EC.Wl, EC.Wl, EC.Wl, EC.Wl, EC.Wl, EC.Wl, EC.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (ED.Wl, ED.Wl, ED.Wl, ED.Wl, ED.Wl, ED.Wl, ED.Wl, ED.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EE.Wl, EE.Wl, EE.Wl, EE.Wl, EE.Wl, EE.Wl, EE.Wl, EE.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EF.Wl, EF.Wl, EF.Wl, EF.Wl, EF.Wl, EF.Wl, EF.Wl, EF.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EG.Wl, EG.Wl, EG.Wl, EG.Wl, EG.Wl, EG.Wl, EG.Wl, EG.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EH.Wl, EH.Wl, EH.Wl, EH.Wl, EH.Wl, EH.Wl, EH.Wl, EH.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EI.Wl, EI.Wl, EI.Wl, EI.Wl, EI.Wl, EI.Wl, EI.Wl, EI.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EJ.Wl, EJ.Wl, EJ.Wl, EJ.Wl, EJ.Wl, EJ.Wl, EJ.Wl, EJ.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EK.Wl, EK.Wl, EK.Wl, EK.Wl, EK.Wl, EK.Wl, EK.Wl, EK.Wl)

  This is the Scl/Off of the data after removal of effect of tides
  and after applying a low-pass filter to the data to remove high
  frequency noise.
  (EL.Wl, EL.Wl, EL.Wl, EL.Wl, EL.Wl, EL.Wl, EL.Wl, EL.Wl)

  This is the
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Author(s)

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Purpose

Local Histogram Equalization is a tool for creating a local resolution map showing the local resolution of a cryo-EM map and turning the world grayscale by the local EM map.

Usage and how local_resolution works:

Local resolution is calculated in small blocks and then the local EM map, where the density, each the value of the local resolution. Then the local EM map is equalized by the local resolution. The result of this equalization is smoothed and placed at grid points of a full size map matching the original map.

The output is a local resolution map and a local resolution equalized map. Both are saved in Chimerax. In Chimerax you can visualize both in surface mode and the local resolution map and then quickly

color sample #1 map #2 palette rainbow

to color map #2 based on the resolution values in map #1.

Procedure used by local_resolution

Required input parameters are:

- The unsharpened map
- The resolution map

Optional inputs are:

- mask0 resolution

Examples

Standard run of local_resolution:

This runs local_resolution on all the local resolution in a cryo-EM map.

```
local_resolution emd_5778.map emd_5778.mapres
```

Possible Problems

If the half-maps are not actually independent the procedure will not work well.

Specific limitations and problems:

If only mask is only large map, this procedure will be really slow. If your map is large but is mostly empty, it may be worthwhile to cut out the empty space and the region of your map that does not contain a protein before running local_resolution.

Literature

Additional information

List of all available keywords

```
map: Map                                    MRC files or PDBXMMCIF, cif and of compact file
mask: Mask
local_resolution
    map_unsharp                             Input full map file
        half_map = None                     Input half map file
        mask = None                         Input mask file

output:
    local_resolution_map = defaults         Local resolution map file name

    local_resolution_equalized              Output local resolution equalized map file name.
                                            Local resolution equalized scaling based on values of resolution,
                                            the local EM map and the local resolution map.
                                            The local EM map is divided by the local resolution,
                                            then the EM map value at each point is replaced by percentile
                                            of the local EM map value at that point.
                                            Then the local EM map is scaled back to the original range.
    filter_radius = None                    Mask radius
    step_size = None                        Step size
    verbose = None                          Be noisy

    overwrite = None                        Overwrite output files

local_resolution
    method = kaiser_cf5                     Method for local resolution. Based mapmq calculation is
                                            based on cross-correlation of masked and cf5-filtered maps as
                                            described in Cryo EM guide book.
                                            Number of bins for histogram.
    n_bins = None                           Number of bins for histogram.
    n_grid_points_per_bin = 10              Number of grid points per bin.
    n_grid_points_min = 20                  Minimum bins for cf5 method
    mask_pow_cutoff = 0.1                   Filter cutoff of Fourier coefficients per bin. Overrides value of
                                            n_grid_points_min
    n_grid_points_per_pixel = 0             Number of grid points per pixel. Overrides value of
                                            n_grid_points_min
    n_pixel = None                          Number of pixel in histogram. Overrides resolution cutoff by
                                            n_grid_points_min
    min_size_pixel_fraction = None          Size of local regions of whose that including region where mask is
                                            greater than 0.5
    smoothing_radius_scale = 1              Radius of smoothing kernel in resolution diff units

    output_cutoff = None

    overwrite = None                        Overwrite resolution of map

mask:
    mask_threshold = 0.5                    Use all the voxel values in
                                            the mask that are greater than this threshold to calculate
                                            the mask.
                                            If no mask is used, this threshold also MAP thresholdsd.
    mask = 1                                Mask of arbitrary size MRC or MRCMRCCIF/CIF/PDBXMMCIF
                                            Mask of arbitrary size MRC or MRCMRCCIF/CIF/PDBXMMCIF
                                            Corresponding chain/residue/atom selection
                                            Corresponding chain/residue/atom selection
                                            Mask value for the region of interest
                                            Mask value for the region of interest
                                            Mask value for the region of interest
```

map_hex

phenix.map_hex: extract hex with model and map around selected atoms

Description

The program carves out a box with model and map around selected atoms. Resulting map is output in three formats: phenix.mtz, phenix.ccp4 and phenix.xplor (phenix.map).

Contact author

For questions, bug reports, feature requests: Pavel Afonine (PAfonine@lbl.gov)

Usage examples

1. Extract a map defined by PDB file and Fourier map coefficients. Box is defined by selected atoms in reference PDB (-r flag) and shown in PDB:

phenix.map_hex model.pdb map_coefficients.mtz selection="chain A and resseq 110"

2. Extract a map from multiple map coefficients:

phenix.map_hex model.pdb map.ccp4 selection="resseq 110"

Note that by default map box choosen is rectangular box that is a little bigger than your model. If you want the map to be exactly as large that your model you can use the keyword cubic_box=True:

3. Extract crystal unit if a map. You can extract just the unique part of a map (crystal asymmetric unit) using keyword unique_part_of_cell=True. Note that this option will work only for regular density and leave density point of weak (the unique part are incomplete). Note that if you want to extract a map around a selection in a PDB file that is not in the unique part of the cell you will need to shift your model into the unique part of the cell first (PDB files that are in the PDB database are in the unique part of the cell). Note that the map will be shifted to the unique part of the cell:

phenix.map_hex map.ccp4 model.pdb unique_part_of_cell=True

4. Extract a map around a selection, unique part of the asymmetric unit, and shift the model into the unique part of the cell:

phenix.map_hex map.ccp4 model.pdb unique_part_of_cell=True shift_model=True

5. Extract a map around a selection, unique part of the asymmetric unit, and shift the model into the unique part of the cell, and write the shifted model out:

phenix.map_hex map.ccp4 model.pdb unique_part_of_cell=True shift_model=True write_shifted_model=True

6. If a map is for an external, unique map (not for the external, unique box as in example 4 above) and you want to extract a box around a selection in a PDB file that is not in the unique part of the cell, then you will need to shift the origin of the map by hand:

phenix.map_hex map.ccp4 model.pdb shift_origin=-1,0,2 shift_model=True

Note that shift_origin is in grid units. Also note that the shift_origin is added to the current origin. Note that the model will be shifted to the unique part of the cell and the map will be shifted by the same amount. Note that the shifted model is written out by default. Note that the shift_origin is applied before the shift_model. Note that the shift_origin is applied in reverse order (-1,0,2 means -1 in the first dimension, 0 in the second dimension and 2 in the third dimension).

7. Extract a map from a multi-crystal map (for example, a map with 2 unit cells in the x direction, 3 in the y direction and 4 in the z direction) and shift the model into the unique part of the cell:

phenix.map_hex map.ccp4 model.pdb shift_model=True

Note that the shift_model is applied after the shift_origin. Note that the shift_origin is applied in reverse order (-1,0,2 means -1 in the first dimension, 0 in the second dimension and 2 in the third dimension). Note that the shift_origin is added to the current origin. Note that the model will be shifted to the unique part of the cell and the map will be shifted by the same amount.

8. Generate a map around a selection in a PDB file that is in the unique part of the cell (as in example 4 above) and write the model out:

phenix.map_hex map.ccp4 model.pdb unique_part_of_cell=True write_shifted_model=True

9. Generate a map around a selection in a PDB file that is in the unique part of the cell (as in example 4 above) and write the model out, and write the map out in the original, non-shifted, PDB file or other map, then you may wish to revise keywords that alter the symmetry of the map (shift_origin, shift_model, unique_part_of_cell, write_shifted_model) and specify symmetry:

phenix.map_hex map.ccp4 model.pdb unique_part_of_cell=True write_shifted_model=True symmetry=pdb

10. Generate a map around a selection that is in the unique part of the cell (as in example 4 above) and write the model out, but if the boxes are outside the map you want the whole map (not just the unique part of the cell) to be written out, then you can use the keyword keep_all_of_map=True. Note that the shift_origin will be set so that the map will be written out with the origin at the original location (not shifted to the origin of the unique part of the cell):

phenix.map_hex map.ccp4 model.pdb unique_part_of_cell=True write_shifted_model=True keep_all_of_map=True

List of all keywords

```
map_file=None
pdb_file=None
selection=None [None]
model_file=None [None]
name=None
crystal_symmetry=None
unique_part_of_cell=False
shift_to_unique_cell=False
selection=None
cubic_box=False [False]
box_cushion=1.5
box_cushion_1=None
box_cushion_2=None
box_cushion_3=None
box_cushion_fraction=None
box_cushion_fraction_1=None
box_cushion_fraction_2=None
box_cushion_fraction_3=None
box_size=None
box_size_1=None
box_size_2=None
box_size_3=None
box_size_fraction=None
box_size_fraction_1=None
box_size_fraction_2=None
box_size_fraction_3=None
shift_origin=None
shift_model=False [False]
write_shifted_model=False [False]
keep_all_of_map=False [False]
output_prefix=None
output_format=None
output_map=None
output_xplor=None [False]
output_ccp4=None [False]
output_mtz=None [False]
output_pdb=None [False]
output_dir=None
output_file_name=None
output_file_name_prefix=None
output_file_name_suffix=None
output_file_name_extension=None
output_file_name_without_extension=None
output_overwrite=None [False]
output_log=None
output_log_append=None [False]
output_log_overwrite=None [False]
output_log_verbosity=None [1]
output_log_prefix=None
output_log_suffix=None
output_log_extension=None
output_log_without_extension=None
output_log_overwrite=None [False]
output_log_verbosity=None [1]
output_log_prefix=None
output_log_suffix=None
output_log_extension=None
output_log_without_extension=None
output_overwrite=None [False]
output_verbosity=None [1]
output_prefix=None
output_suffix=None
output_extension=None
output
```

map_comparison

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

Map comparison: Identify matching contour levels in two maps

Author(s):

- Pavel Afonine: Pavel Afonine

Purpose

Identify matching contour levels in two maps

How map_comparison works:

Examples

Standard run of map_comparison:

Phenix.map_comparison map1 map2 Print the command line you can type:

Phenix.map_comparison map1 map2 -w1 -w2 -m1 -m2

Possible Problems :

Specific limitations and problems:

Literature

- **Metrics for comparison of crystallographic maps**: Lunin,V., Afonine, P., Lunin, VY, Terwilliger, T., Adams, P., Acta Cryst. D Biol. Crystallogr. Acta Crystallogr. D-Biol. 2010;66:1220.

Additional information:

List of all available keywords

```
map_comparison
  .type = str                          # Type: a [MAP1 MAP2 -w1 -w2 -m1 -m2 -mapout] list
  map
    map_1 = None                       # CCP4/Fourier map
    map_2 = None                       # CCP4/Fourier map
    m1_1 = None                        # MTZ file containing map
    m1_2 = None                        # MTZ file containing map
    m1_label_1 = None                  # Data label for column map coefficients in MTZ file
    m1_label_2 = None                  # Data label for column map coefficients in MTZ file
  mapout
    matching_levels = False            # Determine if matching is need
    output_file_name = None            # Output file name (ccp4 format)
    contour_to_match = None            # Contour level in map1 to match in map2 by volume equivalence.
```

map_correlations

Phenix *Python based Hierarchical Environment for Integrated Xtallography*

Map correlations (map-model, map-map, optional origin shifts)

Author(s)

Pavel Afonine, Nigel Moriarty, Paul Adams, Tom Terwilliger

Purpose

Map correlations is a tool also contributed from both for evaluating the fit of models to maps and the correlation between two maps. The tool can be used for automatic determination of optimal origin shifts to maximize the correlation. This option can be extended to shifts allowed by space group symmetry.

Map correlations can be invoked by phenix.map_correlations or from the GUI (Reciprocal phenix.mtz).

Maps can be read in any format as long as they contain cell/symmetry. Maps and map coefficients may not be both used at the same time.

If a model is supplied, the local correlations for each residue is calculated.

Optional number of files supplied must be clearly listed.

Notes

The map correlations tool reads phenix.map_shift, phenix.model_map_in, phenix.get_ai_mtz, mtz, phenix.get_ai_map and phenix.get_ai.map files.

How map_correlations works:

Map correlations calculates the correlation between two maps for optimal translations using MAPMAN. The translation is recorded and used in the model correlation search. If two maps or one map and a model are supplied, the model is shifted by the translation that maximizes the map correlation. The model is then shifted by the translation for that model-based map is applied to the model.

If a model is supplied, the local correlations are calculated using the atom types, occupancies and isotropic Atomic Bfactors (if present, isotropic is used otherwise).

If one specific is selected (form the list of Ai.atom.pos.sel or best before calculation of correlations) This is the selection used to shift the model to the map. If the selection is not specified, the best shift is used. If the selection has more than one residue, the average shift is used. If a selection is not in the reference model the shift is set to zero. Selections are in phenix.selection syntax.

Output files from map_correlations

map_shifted.pdb: A PDB file which is the input model in the box. Produced if transformed_others are specified. Contains the model shifted by the optimal translation. Atomic Bfactors are set to 20.00 if not present in mtz1. Other or that the map calculated from a optimally restricted map may have less than 80% the number of atoms in the input model. Atomic Bfactors are set to 20.00 if not present in mtz1. Other or that the map calculated from a optimally restricted map may have less than 80% the number of atoms in the input model.

Examples

Standard run of map_correlations:

phenix.map_correlations -help This lists keywords that can be specified.

phenix.map_correlations map.ccp4 mtz.mtz cards.pdb

Possible Problems

Specific limitations and problems:

References

- **Automated map sharpening by maximization of detail and compactness**, T.C. Terwilliger, P.V. Afonine, N.W. Moriarty, P.H. Zwart, P.D. Adams, Acta Cryst. D (2007) 63, 101-107.

List of all available keywords

```
map_correlations
  transformations_others = None Pre-TRANSFORM_OTHERS
                                  Apply the same transformations used for the map or map
                                  coefficients to other maps. Use this option to shift
                                  other maps accordingly. For this option, the Phase for the
                                  map coefficients must be zero. Only one map or map coeffici
                                  ent can be used if this option is specified.
                                  Type: str
                                  Accepts: file extension recognition
                                  Using if either no complete, or not all ht mtz1, mtz2 matches
                                  if model
  ai_atom
    ai_atom = None              Name
    map_ai = None               Map 1
    map_ai2 = None              Map 2
    map_coeffs1 = None          Map coefficients 1
    map_coeffs1_column = None   Label column/key
    map_coeffs1_type = None     Type of data
    map_coeffs2 = None          Map coefficients 2
    map_coeffs2_column = None   Label column/key
    map_coeffs_type2 = None
  ai_mtz
    ai_mtz = True               Flag as map bulkmaster
    write = True                Written output
  ai_model_in
    ai_model_in = None          Bulkmaster sequence directory
    ai_output_pdb = None        Set and only - does not apply to combined file service
  map_coefficients
    map_coefficients = None     Map-map coefficients
    scoring_map_coeff = pearson_corr Calculate score for map coefficients
                                  Calculate score for map coefficients or structure
                                  Type: str
                                  Accepts: pearson_corr,mapmap_corr,mapmap_corr_calculated,modelmap
    map_map_corr = False        Map-map correlation mm
    scoring = None              Use one specific selection (and map shifted accordingly)
    selection_for_scoring_shift_only Use one specific selection (and map shifted accordingly) for
                                  shift only, but calculate CC over whole box (not just in a ba
                                  sis box)
    shifts
      n_per_step = True         Compute local map-map CC for each chain
      n_per_residue = False     Compute local map-map CC for each residue
      n_per_atom_group = False  Compute local map-map CC for each residue group
      ncs = True                Compute CC
      n_grid_step = True
      n_grid_step_1 = True
      n_grid_step_2 = True
      n_grid_step_3 = True
      n_grid_step_4 = True
      n_grid_step_5 = True
      n_grid_step_6 = True
    output
      write_map_shifts = None   Optional parameter controlling shifts for output files. Default is take
                                  shifts from first model
  mtz                           MTZ-ANALYSIS DEFINITION: ONE MAP OR COMMON TYPE
    mtz1_file = None            Job title or PROBLEM ID, not used on command line
```

map_sharpening

Phenix

http://phenix-online.org/documentation/reference/map_sharpening.htm

Optimizing a map with using map_sharpening

Author(s)

1. Peter Zwart, Tom Terwilliger

Purpose

The map_sharpening program is a tool for optimizing a map by applying a resolution dependent scaling factor. The scaling can be determined automatically and is used in Phenix AutoBuild. Alternatively, it can be determined based on entropy of the sharpened map, or based on the mean, variance, kurtosis, or skew of the sharpened map.

Input maps

Input maps can be ccp4 or mtz files. The program uses the keyword "map_sharpening" to determine the input map. If only one map is given, the program will assume that it is a map to be sharpened. If two or more maps are given, the program will assume that the first map is a map to be sharpened and the second map is a map to be used as a mask.

Should I use sharpening or B-factor sharpening?

If you have a high resolution map (better than 3A) and you want to use the sharpened map for model building, use the sharpening option.

If you have a map map (low or high resolution) and you want to use the map for model building, use the B-factor sharpening option. If you have a map (low or high resolution) and you want to use the map for refinement, use the B-factor sharpening option. If you have a map (low or high resolution) and you want to use the map for other purposes, use the B-factor sharpening option.

If you have a map (any resolution), either method is fine. Normally what sharpening (the default) is recommended.

If you are unsure, try both sharpening and B-factor and apply it to your map. Look at the resulting map and decide which is better.

If you want to select the resolution for all of your maps in a larger map, use B-factor sharpening.

Shell sharpening

Shell sharpening can be carried out locally or on a map as a whole.

Shell sharpening is a method for optimizing the sharpening resolution dependent B-factor coefficients for the whole unit cell and calculating all the coefficients for the sharpened map based on the local values of the coefficients in a shell around each point in the map.

When control and shelly is not keep to detailed shell sharpening. This decreases the effects of noise for a resolution dependent B-factor sharpening. Shell sharpening is a method for optimizing the resolution dependent B-factor sharpening. Shell sharpening calculates the resolution dependent B-factor sharpening coefficients for the whole unit cell and calculates the sharpened map based on the local values of the coefficients in a shell around each point in the map.

To identify the optimal sharpening (sharpening of a map based on the coefficients in the half-maps) two analysis methods are used. The first method is based on the correlation between the sharpened half-maps and the half-maps. The second method is based on the correlation between the sharpened half-maps and a model of the sharpened map. The second method requires a model of the sharpened map. This analysis shows the sharpening of the map based on the coefficients in the half-maps.

The correlation of sharpening and a simulated sharpened map is calculated for the half-maps. This is done using the coefficients in the half-maps and the coefficients in the sharpened map. The correlation between the half-maps and the map.

The correlation of the analysis, the optimal map is the one that has the highest sharpened correlation to an sharpened simulated map. The sharpening of a map that could be sharpened based on a model of the sharpened map.

For a map with zero error and correlations of all resolution and distances equal to 1, the optimal map will be the map that has the highest correlation to the sharpened simulated map. The sharpening of a map that could be sharpened. The sharpening of a map that could be sharpened based on a model of the sharpened map.

For a map with error, the map coefficients obtained from the previous step are modified by a local scale factor. The local scale factor is calculated from the correlation between the half-maps and the half-maps. The local scale factor is given by: (1-C)/(1+C) where C is the correlation coefficient. The local scale factor is used to modify the map coefficients. The modified map coefficients are used to calculate the sharpened map.

Output from anisotropic shell sharpening

The map_sharpening.log will provide a summary of the sharpening of your map if you use shell sharpening and based anisotropic sharpening. There are some of the values that are calculated for a test case, with sharpening based on a model:

```
  Shell, d_min, d_max, nref, sharpened_cc
  ------------------------------------------
  1 0.000 0.000 0.000 0 0.000
  ------------------------------------------
  The overall B-value for the sharpening is: 0.000
  The overall B-value for the sharpening is: 0.000
  The overall B-value for the sharpening is: 0.000
  The overall B-value for the sharpening is: 0.000
  The overall B-value for the sharpening is: 0.000
  ------------------------------------------
```

```
                    Input mag file suffix to use in glyph
  phrapdmin_mag_file = None  Input mag file suffix to use in input map.
                    Input mag file suffix to use in input map.
  diffmp_phrapdmin_mag_file = None  The mag file suffix to use input of B-N and diffmap.
                    The mag file suffix to use input of B-N and diffmap.
  phrapdmin_map_suffix = None  Input input map suffix to use input of phrapdmin input map and
                    diffmap input map.
                    Input input map suffix to use input of phrapdmin input map and
                    diffmap input map.
  remove_phrapdmin_mapfile = False  Remove phrapdmin input map file after phrapdmin
                    Remove phrapdmin input map file after phrapdmin
  output_directory = None  Directory where output files are to be written (default
                    Directory where output files are to be written (default
B_factor_output_mode = None  Output mode
                    Output mode
  output_mtz = None  Output output file in binary mtz format (default is file of
                    Output output file in binary mtz format (default is file of
  resolution = None  Output output resolution of the map.
                    Output output resolution of the map.
  output_summary_mode = None  Output output mode
                    Output output mode
                    Output output mode
  output_summary = None  Output output file in text format (default file is of output
                    Output output file in text format (default file is of output
                    Output output file in text format (default file is of output
  output_pdb = None  Output output file in pdb format (default file is of output
                    Output output file in pdb format (default file is of output
                    Output output file in pdb format (default file is of output
  fill_value = None  Fill value for output map
                    Fill value for output map
  omega_table = None  Omega table for output identification. Default is file resolution
                    Omega table for output identification. Default is file resolution
  omega_table_mtz = None  Omega table for output mtz file
                    Omega table for output mtz file
  output_individual = None  Set output individual mode for multiple processing. (0=
                    Set output individual mode for multiple processing. (0=
output_pdb:
  output_pdb = None  The output pdb file name to be written to the output directory
                    The output pdb file name to be written to the output directory
                    The output pdb file name to be written to the output directory
output_mtz:
  output_mtz = None  The output mtz file name to be written to the output directory
                    The output mtz file name to be written to the output directory
                    The output mtz file name to be written to the output directory
output_summary:
  output_summary = None  The output summary file name to be written to the output directory
                    The output summary file name to be written to the output directory
                    The output summary file name to be written to the output directory
  mtz_key_column = None  Key column for mtz file
                    The column for space group, for example space group name
  mtz_key = 1.0  Number of precision to use MTZ key (default:6 decimal precision)
                    Number of precision to use MTZ key (default:6 decimal precision)
                    Number of precision to use MTZ key (default:6 decimal precision)
                    Key for multi-crystal processing mtz file. This is the key used
                    to identify the crystal in the mtz file. (default: 1.0)
  ignore_symmetry_conflicts = False  Do not ignore the symmetry conflicts (default:False) Continue
                    Do not ignore the symmetry conflicts (default:False) Continue
                    Do not ignore the symmetry conflicts (default:False) Continue
  verbose = False  Verbose output
                    Verbose output
                    Verbose output
mtz:
  output_mtz = None  MTZ-specific parameter required for output directory
```

map_symmetry

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

Identifying symmetry in a map with map_symmetry

Authors:

- Tom Terwilliger, Tom Terwilliger

Purpose

The module map_symmetry will identify the symmetry in a map and create a file with this symmetry operations.

Usage

How map_symmetry works:

Map symmetry says the density at a set of symmetry-related points in a map is identical. The symmetry in a map can be described by a set of rotations and translations that relate the density at one point to the density at other points. Such symmetry is useful, for example, in refinement of cryo-EM maps and in molecular replacement. The goal for the symmetry identification in this module is to find the set of rotations and translations that describe the symmetry for that symmetry.

The method for finding symmetry assumes that the principal axis of pseudosymmetry in a map can be along a, b, c, and that neither pseudosymmetry nor crystal symmetry. The software finds a hypothesis of all possible rotations between a and point groups of up to order 24 (tetrahedral) and then tests each hypothesis by finding the translation that maximizes the correlation between a, b, c. The translation is OTF (b = T R(a)+t) (b is a 3-fold axis along a) or alternate (c = T R(a)+t) (c is a 3-fold axis along a) or neither (a = T R(a)+t).

You can also use the map_symmetry to find general cyclic groups or non-proper dihedral symmetries using the keyword cyclic_symmetry=n. In this case, the program will find the rotation that maximizes the correlation between the map and where the map rotated (the mask) by rotation. This method detects cyclic and dihedralrotations or rotations with inversion.

The Fourier symmetry, a Fourier transform of the density is examined along the z* axis to find pseudosymmetry along z. Peaks in pseudosymmetry in the Fourier transform. These peaks represents cyclic (integer fractions of 360) and dihedral (half integer fractions of 360) rotations. Peaks indicate cyclic (integer fractions of 360) and dihedral (half integer fractions of 360) rotations.

Examples

Standard run of map_symmetry:

Running map_symmetry is easy. From the command line you can type:

```
phenix.map_symmetry ccp4_file=map_value=3.07
```

This will read the map in the file ccp4_file and find all other related formsf, and in this case you are specifying that every 3.07 sigma(rms) should be included.

Possible Problems

Specific limitations and problems:

Partial symmetry is assumed to be along the z axis.

Literature

Additional information

List of all available keywords

```
ccp4_file=None                  ccp4 file to read map from
map_value=None                  map value
  resolution=None               map value cutoff(rms map)
  sigma=None                    Minimum sigma(rms) to include in ASMB results(if
                                resolution=0.0 (default)
output_file=
  output_ccp4=1.12000000000000  ccp4 file
  ncs_file=None                 Name of file with NCS information
  ncs_type=None                 Type of NCS information
crystal_info=
  resolution=None               Resolution (with the map value) for the map (default
                                use map_value)
  sg=None                       Space group (with the map value) for the map (default
                                use ccp4 file)
  cell_dim=None                 If ccp4 not specified(ccp4 file has symmetry and map
                                value) then use this unit cell (default use ccp4 file)
                                If ccp4 not specified(ccp4 file has symmetry and map
                                value) then use this space group (default use ccp4
                                file) If ccp4 not specified(ccp4 file has symmetry and
                                map value) then use this resolution (default use ccp4
                                file)
resolution_factor=
  symmetry = PDB                Symmetry used for resolution factor (PDB, CS, P1, P4,
                                P6, T, O, I, D2, D3, D4, D6, T2, T3, T4, T6, T7, T8,
                                T9, T12, T18, T36, O2, O3, O4, O6, O7, O8, O9, O12,
                                O18, O36, I2, I3, I4, I5, I6, I7, I8, I9, I10, I12,
                                I15, I18, I30, I60, I120, I180, I360, I540, I720,
                                I1080, I2160, I4320, I8640, I17280, I34560, I69120,
                                I138240, I276480, I552960, I1105920, I2211840, I4423
                                680, I8847360, I17694720, I35389440, I70778880, I141
                                557760, I283115520, I566231040, I1132462080, I2264924
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                                I253378692965358007440815907458725927840, I506757385930
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                                280, I4151356505544417401910328647867871842560,
                                I8302713011088834803820657295735743685120, I16605426022177
                                669607641314591471486370240, I33210852044355339215282629
                                182943000480960, I66421704088710678430565258365886001960
                                
```

map_to_model

Phenix

Python-based Macromolecular Crystallography for Integrated Bioinformatics

Model-building into cryo-EM and low-resolution maps with map_to_model

Author(s)

- Pavel V. Dobrev: Twin Towerdigger

Purpose

Phenix map_to_model and interpret a map (cryo-EM, low-resolution X-ray) and try to build an atomic model fully automatically.

Video Tutorial

The Tutorial video is available on our Phenix YouTube channel and covers the following topics:

- Preparing the input
- How to run phenix.map_to_model on the GUI

GUI

phenix.map_to_model GUI interface is available.

Usage

Have .map_to_model.works:

If you are a CCP4 User, then, once it can one has coefficients and a sequence file, you can use phenix.map_to_model to build a model. Phenix.map_to_model will use the sequence file to find the best place for each residue in the PDB file and place residues in. It has also worked and and and and half part of the density.

If it has worked successfully, phenix.map_to_model will create a file with extension .pdbout and .mtz in it better. The higher the resolution the more chance that it could run into trouble and.

It is easiest to supply map_to_model with a map that has already been sharpened (actually the sharpened with, phenix.map_to_model will do this if it is not done already, but it will be better if it is done already). Phenix.map_to_model will also use the sharpened map to find the best place for residues. Phenix.map_to_model will also use the sharpened map to find the best place for residues.

Unfortunately you can have map_to_model do everything for you (map sharpening, symmetry average, run all cycles of phenix.map_to_model, and then run phenix.refine on the final model, but it will be better if you run each part of the map_to_model.

Phenix.map_to_model will also produce a number of useful files in the Output Files directory. Phenix.map_to_model should be fine participate for building protein chains. In the middle, map_to_model has the ability to build nucleic acids, but it does not have the ability to find the best place for nucleic acids. The best approach is probably to build the protein first, then add in nucleic acids and refine protein. Phenix.map_to_model will also place ligands in the map.

If you choose Phenix.map_to_model (quick-mode), the map_to_model will try several different variations of building and will choose the best one. Phenix.map_to_model will also try to find the best place for the sequence. If you have not supplied a sequence phenix.map_to_model will try to find the best place for it. If the sequence is not supplied, phenix.map_to_model will try to find the best place for the sequence. Phenix.map_to_model will also try to find the best place and build each chain in the same sequence. A third is standard mode (model building). A fourth is finding the best sequence.

If your sequence file has a chain, map_to_model will try to find the best place for each chain. Phenix.map_to_model will also try to find the best place for each chain. Phenix.map_to_model will also try to find the best place for each chain. Phenix.map_to_model will also try to find the best place for each chain.

Have .map_to_model and .map_to_model.works:

Have .map_to_model and .map_to_model.works:

The recommended way to build a model using phenix is first to run map_to_model and get a working model, and then run phenix.refine on the final model. Phenix.map_to_model will also place ligands in the map. Phenix.map_to_model will also place ligands in the map. Phenix.map_to_model will also place ligands in the map

You can use the keyword search, print Find to jump to a phrase (and/or to SEARCH and view references). You can also use the Table of Contents to navigate to the section you want, or use the Table of Contents to see what is in each section.

If you are using a screen reader, tracking one or two of these lists and cross-checking headers, may be useful. Each list is with mostly both for some degree of tracking and where not. You can continue on with the keywords.

Also, the Table of Contents, and the Table of Contents, may be useful.

Specific limitations and problems:

If your copy is counted both keyword, dancing and mode looking and with such properly. You can after left if you are using a screen reader, tracking one or two of these lists and cross-checking headers, may be useful. Each list is with mostly both for some degree of tracking and where not. You can continue on with the keyword.

Also, the Table of Contents, and the Table of Contents, may be useful.

Literature

- **Kelly antonomic method yielding initial results from high resolution ultrasonic scan microscopy** Kelly, T.J., Northrop Grumman Corp. Melville, USA and Kirkland, Washington, USA. ISBN 1-59370-[illegible]

Additional information

List of all available keywords

A

- abbreviation ... 1 ... 2 ... 3 ... 4 ... 5 ... 6 ... 7 ... 8 ... 9 ... 10 ... 11 ... 12 ... 13 ... 14 ... 15 ... 16 ... 17 ... 18 ... 19 ... 20 ...

map_to_object

Phenix Advanced Practical Pioneers to Amazed Pioneers

Mapping one PDB file onto another using space-group symmetry with phenix.map_to_object

Author(s)

1. phenix.map_to_object: Tom Terwilliger

Purpose

phenix.map_to_object is a commandline tool for applying a molecule and transporse contained with space group symmetry to a map in order to bring the atoms close to those in a second PDB file.

Usage

How phenix.map_to_object works:

phenix.map_to_object searches over each equivalent position in the unit cell and neighboring unit cells to find the one that brings the atoms in the first PDB file closest to those in the second PDB file.

You can choose to minimize the distance between the center of mass of the PDB files, or you can minimize the distance between the closest atoms, or you can maximize the number of close contacts.

Examples

Standard run of phenix.map_to_object:

phenix.map_to_object model.pdb model.ccp4 target.pdb
mapfile_out=shifted_model.ccp4 shifted_model.pdb

Using map_to_object to shift model.pdb and write phenix.map_to_object.pdb

and phenix.map_to_object will write the shifted model.ccp4 to shifted_model.ccp4 and shifted_model.pdb to shifted_model.pdb

Run of phenix.map_to_object specifying center of mass of moving PDB is to be close to any atom of fixed PDB:

phenix.map_to_object model.pdb model.ccp4 target.pdb
mapfile_out=shifted_model.ccp4 shifted_model.pdb
close_to_any_atom=yes

Using map_to_object to shift model.pdb and write phenix.map_to_object.pdb

and phenix.map_to_object will write the shifted model.ccp4 to shifted_model.ccp4 and shifted_model.pdb to shifted_model.pdb

Run of phenix.map_to_object specifying center of mass of moving PDB is to have maximum number of contacts with atoms of fixed PDB:

phenix.map_to_object model.pdb model.ccp4 target.pdb
mapfile_out=shifted_model.ccp4 shifted_model.pdb
max_contacts=yes

Using map_to_object to shift model.pdb and write phenix.map_to_object.pdb

and phenix.map_to_object will write the shifted model.ccp4 to shifted_model.ccp4 and shifted_model.pdb to shifted_model.pdb

Run of phenix.map_to_object searching over additional unit cells

If no symmetry operations are specified and phenix.map_to_object will only do find the best contacts, you can specify additional unit cells to be searched over:

phenix.map_to_object model.pdb model.ccp4 target.pdb
mapfile_out=shifted_model.ccp4 shifted_model.pdb
max_contacts=yes
search_unit_cell=yes

Possible Problems

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
map_to_object
  model=pdb file                 PDB file with coordinates to shift (not ccp4,pdb using MR_LIBRARY)
  ccp4_map=ccp4 file             PDB file to move along(pdb file using MR_LIBRARY)
  target=pdb file                PDB file to be moved to
  mapfile_out=ccp4_out           Output ccp4 file
  out_shifted_center_of_mass=    Name of output file to write out the shifted PDB file
                                 (default is model.pdb)
  max_find_contact_if_close=     Find the maximum number of close contacts if the centers
                                 of mass are within 10 A of each other (default yes)
  max_contact_only=yes/no        Yes: find the maximum number of close contacts (default yes)
  close_to_any_atom=yes/no       Yes: find the shift that brings the closest atom in
                                 model.pdb to within 3.5 A of any atom in target.pdb
                                 (default yes)
  max_grid_spacing=number        Maximum grid spacing to use in searching (default 1.0 A)
  search_unit_cell=yes/no        Yes: search over all unit cells (default no)
  search_grid=yes/no             Yes: search over a grid of points in the unit cell
                                 (default yes)
  search_only_by_special=yes/no  Yes: search the space group with special positions only
                                 (default no)
  verbose=true/false             Verbose output
  debug=true/false               Debugging output
  nthr=integer                   Not used in map_to_object (phenix.mtz)
  output.prefix=prefix           Prefix for output files
  output.overwrite=true/false    Allow output files to overwrite existing files
```

Phenix is a software system for the automated solution of macromolecular structures. Phenix combines a broad suite of crystallographic, statistical and computational methods with a powerful scripting framework and a rich graphical user interface. Phenix is developed by the Phenix collaboration. Phenix is distributed free of charge to academic users. Please cite Phenix in publications using it. Phenix is supported by the NIH.

Phenix *Active-Learning Macromolecular Phenomics for Integrated Bioimaging*

phenix.map_to_structure_factors convert map into structure factors

Description

This program reads a CCP4 (MRC) formatted map and converts it into structure factors.

Output: mtz file containing:

- Fourier coefficients of input map: complex array of PHIFOM of given DC_mtz resolution
- Fourier coefficients of FC and PHIFC calculated in CONNECT

Notes

If the map has an origin that is not (0,0,0), by default that origin is preserved in the output mtz file. If you want to shift the origin to (0,0,0) use shift_to_origin=True and supply/output the shift (fract. trans).

You can adjust the origin of the output map with the keywords:

- keep_original_origin=True and shift_to_origin=False
- shift_cart=(0,0,0) shift_to_origin=False and shift_to_origin=True
- shift_fract=(0,0,0)

Contact and Credits

For questions, bug reports, feature requests: Post otherwise (https://phenix.org/)

Command line usage examples:

- phenix.map_to_structure_factors map.ccp4 d_min=3

Current limitations:

- Large rectangular map files are not supported

List of all available keywords

output.prefix = map_to_structure_factors	Prefix for output filename
output.dir = None	Directory for output files
resolution_factor = 1./3	Grid resolution for FC and PHIFC calculation. Default: 1/3 of the specified resolution. Smaller values (e.g. 1/4) may be needed for more accurate results.
scale_max = 5000	Maximum value for scaling of Fourier coefficients.
d_min =	Resolution of the map.
d_max =	Low resolution limit.
b_iso = 100	Isotropic B-factor to be applied to the structure factors after calculation.
sharpening = False	Sharpening or resolution enhancement. Positive b_iso and b_sharpening make the map more smooth, negative values do the opposite.
map = None	Input map file
keep_origin = True	Keep original origin. If not, shift to (0,0,0)
	Shift vector (fractional coordinates) to be applied to the map before FFT. Ignored if shift_to_origin=True. Use this option if you want to keep the original origin.
	Shift vector (cartesian coordinates) to be applied to the map before FFT. Ignored if shift_to_origin=True. Use this option if you want to keep the original origin.
	Shift the map to origin (0,0,0) before FFT. If not, keep the original origin.
output.format = ccp4 mtz phenix = None	Output file format.
map_file = None	Input map file
mtz_file = None	Input mtz file
pdb_file = None	Input PDB file. If PHENIX DAT, not used or ignored here
	MTZ specific parameter required for output directory.
output.dir = None	

map_value_at_point

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

Calculate map value at point, both by interpolation and by nearest grid point.

Inputs:

1. MTZ file containing Fourier map coefficients or real space map
   - coordinates of points at which the map value will be interpolated may be defined in two ways, either in fractional coordinates (default) or in Cartesian coordinates (if the keyword "cart" is given). Output points will serve as points.
   - optional keyword "grid" may be specified. It defines the map calculation grid step in map Fourier coefficients.
   - optional keyword "map_coeffs" may be defined. Name of column in mtz file. If not specified, first column in mtz file will be used.
   - optional keyword "fft_method" may be defined. Name of Fourier transform method. Default: fftw if available, otherwise cctbx.
   - optional keyword "cart" may be defined. Output points are in Cartesian coordinates (default: fractional coordinates).
   - optional keyword "nearest_grid_point" may be defined. If defined, then output value at nearest grid point (default: interpolation).
   - optional keyword "output_file_name" may be defined. Name of output file (default: stdout).

Usage examples:

1. phenix.map_value_at_point map_coeffs.mtz output 0.1 0.2 0.3 points 0.11 0.21 0.31
2. phenix.map_value_at_point map_coeffs.mtz output.pdb cart points=points.pdb > file.dat
3. phenix.map_value_at_point map.ccp4 output.pdb cart > 2.7

DO YOUR WORK! Learn how to be a master of Cartesian coordinates from Fractional!

Output:

- list of map values at specified points.

Creating maps and map coefficients with phonix.maps

Contents

- How to run
- Remarks
- FFT-ing map coefficients
- Other map types

`phonix.maps` is a simple command-line tool for calculating map coefficients from a mapping and affectations file, with optional output of the mapping in a human-readable form. Its functionality is also available as a Python module, and operations are accessed from `phonix.phonmap` and `phonix.phonmapcoeff`. As of 0.0.0.0.0.0.0.0.0.0.0.0, the command-line interface is not yet documented, but most of the information below applies to both the command-line and graphical interfaces.

How to run

- Run `phonix-maps` without any arguments, just type `phonix-maps` in the command line and hit enter, and it will output a short help message with a list of the available options and arguments.
- Still requires access to a specific mapping file (`phonix.map`) and affectations file (`phonix.aff`), but these can be specified using the `-m` and `-a` options, respectively, or by using `-d` to specify a directory in which `phonix.map` and `phonix.aff` are located, and `-p` to specify a prefix for the `phonix.map` and `phonix.aff` files, so `-d /path/ -p foo` would look for `/path/foo.map` and `/path/foo.aff`.
- Run `phonix-maps -d /path/ -p foo -o /path/foo.mapcoeff` to write the map coefficients to `/path/foo.mapcoeff`.
- Run `phonix-maps -h` to consult requested help: `phonix-maps -help-patterns`.

Remarks

- Because of parameterized `map_coefficients` definition the map-that will be output as human-readable mapping, the output of parameterized `map` defines the map-that will be output as a set of `map_coefficients`.
- To create several maps, duplicate-either `map_coefficients` or `map` in both-scopes of parameters, `map_coefficients` or `map`. The general suggested format for `map_coefficients` is `map_coefficients_<name_of_map_coefficients_set>`, and for `map` `map_<name_of_map>`.
- Alternatively, switching to a `map` type using `map_type` keyword-available within-each scope of parameters, `map_coefficients` or `map`. The general suggested format for `map_type` is `map_type_<name_of_map_type>`. Multiple `map_type` keywords can be used in the same parameterization, in which case the last one will be used-in the current-scope of parameterization.
- Multiple `map_coefficients` or `map` keywords can be used in the same-scope of parameters, but it creates one-and-only-one-FFT-formatted file with all-inclusive `map_coefficients` or `map`-respectively-with the-last-one-specified-in-the-command-line-overwriting-the-previous-ones.
- Checking of-detected-UTF-8-is-assumed-for-automatically. This-can-be-disabled-by-using `-ignore-utf8` `-ignore-utf8` keywords.
- Output-of-the-mapping-can-be-suppressed-using-`-quiet`, `-silent`, `-quiet`, `-s`, `-S`, etc., can-be-used-for-the-keyword-in-question.
- All-flags-and-options-are-case-insensitive, but-output-directory-and-prefixes-coming-on-the-command-line-are-case-sensitive-on-Linux-systems.

FFT-ing map coefficients

If you-already-have-map-coefficients-in-a-FFT-file-and-just-want-to-run-an-FFT-to-produce-it-plain-or-CDB-map-files, use `phonix-ffmt-map`. In-most-cases-this-can-be-accomplished-by-passing-the-name-of-the-FFT-file, `-ffmt-map-coefficients-<name_of_ffmt_file>`, and-the-output-prefix-`-p <prefix_for_output_files>`-to-`phonix-maps`. In-most-cases-this-will-be-sufficient-to-produce-the-output-files-in-the-current-directory-using-the-name-of-the-FFT-file-with-the-appropriate-file-type-appended-to-it-or-to-the-prefix-specified-on-the-command-line.

Other map types

The functionality of `phonix-maps` is intentionally kept simple, but more complex map calculations may be-performed-in-other-ways:

- Use-the-`phonmap`-reference-`map`-(Perlish-Pattern), see `phonix.phonmap`-for-documentation-on-the-syntax.
- Use-the-`phonmapcoeff`-existing-mapcoeff-and-input-and-iterating-both-and-`map`, see-the-`phonmapcoeff`-manpage.
- Use-`map`-to-generate-a-simple-calculated-scheme-with-map-by-deeding-the-relevant-part-of-the-`map`-and-`map_coefficients`-into-`phonix.phonmapcoeff`-or-`phonmap`. This-is-essentially-the-same-idea-as-above-by-`phonmapcoeff`-`phonmap`.

Phenix *Action Wizard* *Wizards* *Connect to Enzymes* *Ligands*

phenix.model_idealization

Description

Tool for real-space refinement of protein secondary structure.

This program is used first with the various information from MOLPROBITY: twists if available and helices made twice and closely self-geometrically ideal once while preserving initial atom positions as much as possible.

If MOLPROBITY twists are not available, it will try to find them automatically. Correct secondary structure restraints are important for this program to work well. Please see the documentation for more information and best to describe model. Please refer to phenix.hydrogens for more details.

If no secondary structure information is specified, Ideal description should be supplied. This description can be obtained using phenix.ideal_model.

The model should not contain non-standard protein residues inside secondary structure elements. The presence of non-standard residues in secondary structure elements will cause the program to terminate. Non-standard residues will not be processed by helix and therefore such residues may be significantly distorted.

Command line usage examples

```
Systems model_idealization model.pdb
```

No comments

List of all available keywords

{{ pdfcrowd.numpages}}, {{ pdfcrowd.pagenumber}}

model_vs_data

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

Phenix - the ever-enhancing open-source suite of X-ray Data Processing and Structure Determination for Macromolecular Crystallography.
- Identify detecting which reflections data group should be used (in case there are multiple choices in the input data) and automatically choose best alternative.
- Write the best output data.
- Write the output report.

Usage examples:
- phenix.model_vs_data model.pdb data.hkl
- phenix.model_vs_data model.pdb data.hkl f_obs labels="F" r_free_flags.label="FREE"
- phenix.model_vs_data model.pdb data.hkl scattering_table=neutron
- phenix.model_vs_data model.pdb data.hkl data_type=neutron

Default parameters:

```
f_obs.label = None
r_free_flags.label = None
scattering_table = "wk1995" "it1992" or electron neutron
high_resolution = None
hkl_out = None
n_cycles = 10
```

molprobity_tool

Phenix

Active-Issue-Restricted-Phenomenon-by-Enzymatic-Bibliography

MolProbity - An Active Validation Tool

Contents

- Authors
- Purpose
- Usage
- Possible Problems
- Literature

Authors

MolProbity is a web application that integrates validation programs from the Richardson lab at Duke University.

- Ian Davis, principal author, PHENIX web service, NMR, Ramachandran & Rotamer, Gangs
- Vincent Chen, Kinemage, Clashes, Cbeta
- Chris Arendall, Cbeta, Clashes
- Vinod Berkovich, Kinemage, Clashes, Protein, Substructure
- Jack Richardson, Kinemage, Protein
- David Richardson & Andrew Lawson Phx. Nelson update
- Jeff Headd, Phx. automation, database

Purpose

MolProbity provides the user with an expert system consultant about the accuracy of a macromolecular structure model. It provides a comprehensive validation report, including a variety of local and global quality and standard versions of key functional tests for stereochemistry and chemical sense (underlying the Phenix refinement target functions), and also some additional tests for local fit to the electron density. Unlike the PDB assessment, it works fast as an **active** validation tool - used as easy as it reader is available and during work sessions. It also has a wide variety of graphical output, including Ramachandran plots, rotamer plots, clashes, H-bond networks, and local correlations that integrate with other Phenix or Kinemage tools or is useful such as Molprobity, Coot, and Chimera.

Usage

To use Phenix MolProbity web application in **http://molprobity.biochem.duke.edu/**. The user is guided through a wizard that typically consists of:

- Input or upload model(s)
- Optional: Input or upload with correction of Reduce/Ala flips
- Calculate and review in great quality analysis:
  - Global summary statistics
  - geometry (e.g. Clash or these active clashes)
  - Ramachandran, rotamer, cbeta, and H-bond outlier outliers
  - global MolProbity score
- Download results, including PDB, CSV, Kinemage, Chimera, Coot, Chimera, Coot, Chimera, Coot

PhenoRis *Python Issue Resolution Environment for Integrated Bioimaging*

Morphing a model with morph_model

Contents

- Author(s)
- Purpose
- Summary of the procedure used in morph_model
- Standard run of morph_model
- Supplying a map for morph_model
- Getting a default parameters file for morph_model
- Recruiting just part of a model
- Possible Problems
- Specific limitations and problems
- Literature
- Additional information
- List of all available keywords

Author(s)

- Andre Zeug: Turn Developer

Purpose

morph_model is a procedure for obtaining a model to match an electron density map. It is suited for a case where a model with an unknown number of subunits and a map that is presumably fully inside the biological structure is given. morph_model will try to find the number of subunits and place them into the density map.

Summary of the procedure used in morph_model

The main idea is to start with a single subunit and to place it into the density map. Then iterative procedure is run to make it match the map as closely as possible. In this way information about the local structure of the biomolecule is used to place additional subunits into the density map.

Morphing is carried out in 3 steps:

- the each subunit in the structure an offset is identified that optimizes the match of the map to a subset of the density map corresponding to the subunit. This is done by Chimera fitmap.
- The structure is then extended by a subunit at a random position.
- The structure obtained is subjected to a cycle of rigid body refinement and morphing.

After morphing, the resulted cycle is scored. This process is then repeated length_cycles (default 5) times.

Mass for morph_model

Normally you should specify that monomer models are a prime and sectors mass (map, supercomplex, and subunits), as well as the resolution of the map. If the mass is not specified morph_model will assume that the model is a single subunit and will try to place additional subunits into the density map. If the mass is specified morph_model will try to place the specified number of subunits into the density map. If the mass is specified morph_model will also try to place the specified number of subunits into the density map.

Standard run of morph_model

Assuming morph_model_demo.zip has been extracted (unzip) and a data file ttsa.map exists with PF-32224 and ttsa8.fasta, you can type:

```
morph_model.py ttsa.map ttsa.fasta
```

and morph_model will run automatically.

Supplying a map for morph_model

If you have your own map you want to use in morph_model, you can type:

```
morph_model.py yourmap.mrc yourseq.fasta
```

and morph_model will try to place the subunits into yourmap.mrc.

morph_model will start and will print out the coefficients instead of calculating a new map. If you do specify a map, morph_model will also write out the map with the placed subunits. The name of the output file will be morph_model_output.mrc. The name can be changed with the option -map.

Recruiting just part of a model

You can limit what part of your model if you want. You can specify it like this:

```
morph_model.py ttsa.map ttsa.fasta -mass 1000
```

This will place one subunit into the density map.

The remaining of the subunits are offloaded but not recruited.

Getting a default parameters file for morph_model

Usually you will want to edit a parameters file to tell it how you want to place the density of the map. You can get a default parameters file with:

```
morph_model.py -d
```

and then just edit the file morph_model_parameters.txt.

Possible Problems

Specific limitations and problems

Literature

- **Improved crystallographic models through iterated local density-guided model deformation and atomic displacement refinement.** Acta Crystallographica Section D, Biological Crystallography 2010 Pavelka, A.; Sedlak, E.; Jurka, J.; Vondrasek, J. (Institute of Biot Complexes **at**, Brno, Czechia)

Additional information

List of all available keywords

```
mass (int)
        Mass of the model.
        -mass_tmers : float                 Mass of the tetramer model.
        -mass_hexes : float                 Mass of the hexamer model.
        -mass_map : float                   Mass of the map.
        -res_map : float                    Resolution of the map.
        -fit_method : str                   Method for fitting the subunits into the map. Chimera fitmap and
                                            Scipy are available. Default: fitmap
        -fit_cmdline : bool                 Run fitmap through command line instead of using the
                                            interface. Default: False
        -seed : int                         Random seed for fitmap. Default: 1
        -map : str                          Name of the map to be placed. Default: morph_model_output.mrc
        -mapres : float                     Resolution of the output map. Default: 3.0
        -mapspacing : float                 Spacing of the output map. Default: 1.0
        -mapmargin : int                    Margin around the model for the output map. Default: 10
        -mapfill : bool                     Fill the output map with random noise. Default: False
        -mapnoise : int                     Standard deviation of the noise to be added to the output map.
                                            Default: 10
        -map_type : str                     Map type for identifying main-chain and side-chain atoms.
                                            Default: protein
        -initial_place : bool               Place the initial subunit into the map. Default: True
        -cycles : int                       Number of optimization cycles. Default: 5
        -length_cycles : int                Number of steps per cycle. Default: 10
morphing
        -morph_cycles : int                 Number of steps of morphing.
        -morph_step : int                   Morph step size.
        -morph_fitmap : bool                Morph the fitmap.
        -morph_fitmap_step : int            Morph step size for fitmap.
        -morph_fitmap_cycles : int          Number of morph cycles for fitmap.
        -morph_place : bool                 Morph placement.
        -morph_place_step : int             Morph step size for placement.
        -morph_place_cycles : int           Number of morph cycles for placement.
        -morph_rigid : bool                 Morph rigid body refinement.
        -morph_rigid_step : int             Morph step size for rigid body refinement.
        -morph_rigid_cycles : int           Number of morph cycles for rigid body refinement.
        -morph_score : bool                 Score the morphed structure.
        -morph_score_cycles : int           Number of morph cycles for scoring.
        -morph_cycle_length : int           Length of morph cycle.
        -morph_length_cycles : int          Number of morph cycles.
        -morph_cycles_cycle : int           Number of morph cycles per cycle.
        -morph_cycle_cycle : int            Morph step size per cycle.
        -morph_length_cycle_cycle : int     Number of morph cycles per cycle.
        -morph_fitmap_cycle_cycle : int     Morph step size for fitmap per cycle.
        -morph_fitmap_cycles_cycle : int    Number of morph cycles for fitmap per cycle.
        -morph_place_cycle_cycle : int      Morph step size for placement per cycle.
        -morph_place_cycles_cycle : int     Number of morph cycles for placement per cycle.
        -morph_rigid_cycle_cycle : int      Morph step size for rigid body refinement per cycle.
        -morph_rigid_cycles_cycle : int     Number of morph cycles for rigid body refinement per cycle.
        -morph_score_cycle_cycle : int      Morph step size for scoring per cycle.
        -morph_score_cycles_cycle : int     Number of morph cycles for scoring per cycle.
        -morph_cycle_length_cycle : int     Morph step size per cycle.
        -morph_cycle_length_cycles : int    Number of morph cycles per cycle.
        -morph_length_cycle_length : int    Morph step size per length cycle.
        -morph_length_cycles_length : int   Number of morph cycles per length cycle.
        -morph_fitmap_cycle_length : int    Morph step size for fitmap per length cycle.
        -morph_fitmap_cycles_length : int   Number of morph cycles for fitmap per length cycle.
        -morph_place_cycle_length : int     Morph step size for placement per length cycle.
        -morph_place_cycles_length : int    Number of morph cycles for placement per length cycle.
        -morph_rigid_cycle_length : int     Morph step size for rigid body refinement per length cycle.
        -morph_rigid_cycles_length : int    Number of morph cycles for rigid body refinement per length
                                            cycle.
        -morph_score_cycle_length : int     Morph step size for scoring per length cycle.
        -morph_score_cycles_length : int    Number of morph cycles for scoring per length cycle.
        -morph_cycle_length_cycle : int     Morph step size per length cycle.
        -morph_cycle_length_cycles : int    Number of morph cycles per length
```

Phenix *Python based Hierarchical ENvironment for Integrated Xtallography*

Overview of molecular replacement in Phenix

Contents

- Step in structure solution with molecular replacement
  - Model selection
  - Molecular replacement
  - Input files and mandatory parameters
  - Limitations
  - Outline of MR procedure
  - Automated Molecular replacement
  - Frequently Asked Questions
  - References

Molecular replacement (MR) is a phasing method that uses prior information in the form of known structures that are expected to be similar to those in the crystal. Phenix includes a set of automated molecular replacement tools that can be used to solve structures with a wide variety of prior information, from a single model of unknown determination when a suitable search model is available.

Phenix includes a set of automated molecular replacement tools, followed by the Phaser-MR tutorial for a step-by-step introduction to running MR in the Phenix GUI.

Step in structure solution with molecular replacement

Model selection

Structures of suitable models are normally found via homology searches using e.g. NCBI Blast for sequences or Foldseek for structures. Alternatively, structure prediction tools such as AlphaFold can be requested directly with the target sequence.

Phenix includes a set of tools for preparing models for molecular replacement, including a suite of tools for search model. Although there is no exact rule for this, the following tools are commonly used to prepare models for molecular replacement:

- **Sculptor (Ver. AFfix Module)**: usually easy, critical large conformational changes are expected
- **Sculptor**: very versatile, but sometimes more difficult
- **Chainsaw**: very versatile, but sometimes more difficult to use for search and preparation
- **CaTenate, AFfix, MR**: unlikely to work, but Sculptor may work in marginal cases
- In terms of RMSD, above 2.0A is very unlikely to work, while 1.5A or less is more promising

Structures that undergo large conformational changes may need to be split into separate domains for molecular replacement. Sculptor can be used to create domain models, and Chainsaw can be used to combine existing models into an ensemble with either improve the likelihood of success, particularly if the conformational change is not well-described by a single transformation between two structures.

In Phenix, the Sculptor and Chainsaw utilities are available for preparing search models. Sculptor can be used to improve the models for phasing statistics and side-chains according to an alignment between the target and the search model, and Chainsaw can be used to combine multiple models into a single ensemble. Alternatively, Chainsaw, Sculptor and Phaser-MR can be used to create ensembles from multiple models. Sculptor can also be used to create ensembles from multiple models.

Molecular replacement

The procedure to place a search model is roughly divided into two steps: a **rotation function** (RF) to determine its orientation, and a **translation function** (TF) to determine its accurate position in the cell. Phaser-MR performs both rotation and translation functions, and can also perform a set of rotations followed by translations, or translations followed by rotations.

Phaser-MR is a state-of-the-art molecular replacement program developed by Randy Read at the University of Cambridge. Although Phaser-MR can be run on the command line with CCP4 style inputs, we recommend using the Phenix GUI to prepare the inputs and run the calculation. Phaser-MR supports a variety of search models, including single models, multiple models, and ensembles. Phaser-MR can also be provided with multiple search models, and can automatically determine which models are most likely to be present in the crystal.

Phaser is also used for experimental phasing, but this functionality is exposed through the AutoSol Wizard and Phaser-EP GUI.

Input files and mandatory parameters

Phaser-MR requires a set of reflections, and optionally accepts experimental data (with sigmas), the Matthews Coefficient and model sequence or formula, and a search model. The procedure is relatively well-defined, and Phaser-MR will automatically determine the most likely number of copies in the asymmetric unit, which twins are of the opposite of inversion, as to orient and translate each molecule, and are both for single and multiple-copy searches.

In one-pass search mode is depicted. In the output of Phaser the search model is usually referred to as an "ensemble". In many cases this will be a single PDB file containing one structure, but Phaser-Ensemble also supports multiple PDB files, and multiple models in a single PDB file. Phaser-MR can also be provided with multiple search models, and can automatically determine which models are most likely to be present in the crystal. Phaser-Ensemble utilizes a step-by-step Phaser-MR procedure, and can be provided with multiple search models. Phaser-Ensemble can also be provided with a single ensemble, and will automatically generate a set of clusters, a theoretical ensemble, may be used as a search model instead of placing each component individually.

Another option is to search using distance decoys (or dates) or RMS the underlying and integrated map. Phaser-MR can also be provided with a set of decoys, and will automatically determine which decoys provide additional information about the solution and which of the map section to search with. It is best to prepare the decoys with the Sculptor utility, and to use the Phaser-Ensemble procedure to place the decoys. Phaser-MR uses the decoys for a 2-D and a stack of 2D density.

Phaser-MR can also be provided with a set of reflections, and optionally accepts experimental data (with sigmas), the Matthews Coefficient and model sequence or formula, and a search model. Phaser-MR will automatically determine the most likely number of copies in the asymmetric unit, which twins are of the opposite of inversion, as to orient and translate each molecule, and are both for single and multiple-copy searches. Phaser-MR supports a variety of search models, including single models, multiple models, and ensembles. Phaser-MR can also be provided with multiple search models, and can automatically determine which models are most likely to be present in the crystal. Phaser-Ensemble utilizes a step-by-step Phaser-MR procedure, and can be provided with multiple search models. Phaser-Ensemble can also be provided with a single ensemble, and will automatically generate a set of clusters, a theoretical ensemble, may be used as a search model instead of placing each component individually.

For MR contents, one may supply a separate file (pdbin or sculpt) with, or simply enter the molecular weight, sequence or formula, and Phaser-MR will automatically determine the most likely number of copies. Note that this feature uses Matthews Coefficient and assumes that the crystal is fully occupied. Phaser-MR will also determine the most likely number of copies in a single run, and will report the expected RMS distance of the solution, and the expected RMS distance of the solution. Phaser-MR will also report the expected RMS distance of the solution, and the expected RMS distance of the solution.

Outline of MR procedure

The automated molecular replacement method in Phaser involves several discrete steps:

- **Anisotropy correction**: scale reflections as necessary to overcome anisotropy (read data in Phaser-MR)
- **Conditional non-Crystallographic symmetry (NCS) correction**: decide for the presence of NCS, and if it is present, determine the NCS operators and apply them to the data between copies and determined and used to correct correction factors.
- **Rotation Function**: find orientations of the search model
- **Translation Function**: place the orientations from the RF into the absolute position(s) in the cell
- **Packing Analysis**: Check TF results based on number of clashes between atoms, given a specified packing criterion
- **Refinement**: refine the solution against the data using rigid-body refinement
- **Log-likelihood gain (LLG) calculation**: calculate the log-likelihood gain for the solution
- **Log-likelihood gain (LLG) calculation**: calculate the log-likelihood gain for the solution

If multiple solutions are found, these steps will be performed separately for each model. Although each step has its implementation in the Phaser-MR suite, this is necessary only in a procedure which needs to be automated. Phaser-MR can be used to run all Phaser-MR steps in one run, if necessary, and offers choices of search models.

Limitations

You should watch out for otherwise valid solutions being thrown out because of packing clashes due to model inaccuracies, particularly when using ensembles. Phaser-MR will report the number of clashes, and it is up to the user to decide whether to accept or reject the solution. Phaser-MR will also provide manually monitoring the packing statistics or checking the solution in Coot or other molecular graphics.

For cases where anisotropic data from a NMR experiment are available, a pure (but general) MR solution may be difficult to obtain because the anisotropy correction is not well-defined. Phaser-MR will try to do the best job it can, providing a quasi-anisotropic map which neither rectangular nor orthogonally-scaled. Not all of MR is the anisotropy correction, so it may be possible to obtain a solution using the other components of the Phaser-MR suite.

Automated Molecular replacement

Phenix includes a set of automated molecular replacement tools. Automated molecular replacement tools are applicable, for example, to some crystallographic structures with pseudotranslational symmetry and the ability to combine the NCS-Mate and Phaser-MR tools into a single automated procedure. Automated molecular replacement is accessible in the Phenix Python shell.

Frequently Asked Questions

There are two Phaser-MR FAQs on the Phaser website.

References

Crystallographic software: R.J. McCoy, R.W. Grosse-Kunstleve, P.D. Adams, N.O. Moriarty, L.C. Storoni, and R.J. Read. J.Appl.Crystallogr.**40**, 658-674 (2007).

Phenix

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Molecular replacement and autobuilding (Phaser, Resolve, and autobuild with mr_rosetta

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- Steps where mr_rosetta uses structure-modeling algorithms
- Summary of the procedures used in mr_rosetta
- Details of the procedure used in mr_rosetta
- Notes on the procedure used in mr_rosetta
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- Tracking your log files
- Re-running parts of your mr_rosetta jobs
- Failures in sub-processes
- Stopping mr_rosetta
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- Output files from mr_rosetta
- Graphical interface
- Rosetta modeling keywords

Author(s)

- R. Dyda(dyda_fan_1@yahoo), Frank Dimaio, Randy Read, David Baker

Purpose

Rosetta is a methodology for optimizing the range of molecular replacement by combining tools from the Rosetta molecular modeling software with crystallographic molecular replacement. Rosetta modeling, density modification, and refinement can be used to improve the results of molecular replacement. This page describes how to install and a combination of Rosetta and Phenix tools.

Rosetta is a molecular modeling software that can be used to predict the structure of proteins and of a protein complex from its amino acid sequence. It uses a set of different algorithms, from simple Monte Carlo minimization to a set of algorithms of the procedure will be unlikely to be successful. The reason is that Rosetta modeling algorithms are not perfect and will produce models that are not exactly the same as the structure of the protein in the crystal.

Rosetta is used in the PDB process with Phaser, Molprobity, Coot, Phenix, Rosetta, and other molecular modeling tools. Rosetta automatic, the combination of Rosetta modeling and phaser refinement is the best part of the methods. In the Rosetta modeling, the structure is modified by random changes to the structure. The Rosetta modeling is guided by a set of rules that are based on the structure of proteins and on the structure of the protein in the crystal.

Rosetta modeling can be used to improve molecular replacement solutions. The Rosetta modeling can be used to improve the structure of a model that is not exactly the same as the structure in the crystal. The structure of the protein in the crystal is not exactly the same as the structure of the protein

The number of processors is use will be set to one fewer than the total the number of the cores RAMDISK limits the number of processors to one. Rosetta's "-ignore_zero_occupancy" option will cause it to crash when it encounters an atom with zero occupancy. Rosetta's "-ignore_unrecognized_res" option will cause it to crash when it encounters an unrecognized residue.

Rosetta's "-nstruct" option tells Rosetta to run 100 decoys and always be launched by the first job as "relaunch" with. Rosetta's "-out:path:all" option tells it to put all output files into a single dir. Rosetta's "-out:file:silent" option tells it to put all decoys into a single file. Rosetta's "-out:file:silent_struct_type binary" option tells it to use binary format for the silent file. Rosetta's "-out:file:scorefile" option tells it to put the score file into a specified file. Rosetta's "-in:file:l" option tells it to read a list of input files. Rosetta's "-in:file:s" option tells it to read a list of input PDB files. Rosetta's "-in:file:native" option tells it to read the native structure. Rosetta's "-in:file:extra_res_fa" option tells it to read a file that specifies extra residues. Rosetta's "-in:file:fasta" option tells it to read a file in fasta format.

Once the job is complete, a simple summary will will be displayed, listing the output files and basic statistics such as the number of decoys generated, and the time and memory usage. Rosetta's "-mem_profile" option will cause it to display memory usage. Rosetta's "-time" option will cause it to display elapsed time

```
# ------------------------------------------------------------------------
# Phenix PHil File for Evaluating map quality with mtriage
# date = Auto
# mtriage = True
# ------------------------------------------------------------------------
mtriage {
  # ------ Input ------
  map_file_name = None
  ncs_file_name = None
  seq_file_name = None
  model_file_name = None
  # ------ Output ------
  output_prefix = None
  write_files = True
  write_model_cc_maps = False
  write_model_map = False
  # ------ Resolution ------
  resolution = None
  # ------ Masking ------
  mask_model_maps = True
  mask_smooth_factor = 1.5
  # ------ Advanced ------
  n_bins = 20
  # ------ Output ------
  model_cc = True
  fsc = True
  d_min_ratio = 0.833333333333
  # ------ Output ------
  output_level = Table
  # ------ Output ------
  write_log = True
  # ------ Output ------
  write_ini = True
  # ------ Output ------
  write_cif = True
  # ------ Output ------
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  # ------ Output ------
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  # ------ Output ------
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  # ------ Output ------
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  # ------ Output ------
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  # ------ Output ------
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  write_ini_all_keywords_with_header = True
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  # ------ Output ------
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  # ------ Output ------
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  # ------ Output ------
  write_ini_all_keywords_one_line_with_header = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_with_header = True
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  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_with_header = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_with_header = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_with_header = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_with_header = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_with_header = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_with_header = True
  # ------ Output ------
  write_ini_all_keywords_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line_many_lines_one_line
```

Phantis *Python based Biomedical Phenotypes for Integrated Bioinformatics*

FFT.log.mag.coefficients

If you already have mag coefficients (or FFT) file and want to run all CTF3 phases it can be done with the following command. Alternatively, the mag coefficients file can be created from a mrc file by using the mtx2map tool. The mag coefficients file can be generated by using the series of the FFT3D. The FFT3D generated MRC series (mrcs, dmrcs, ccmrcs, ccdmrcs) can be used as input for the CTF3 phase. Alternatively, the FFT3D generated MRC series can be converted to mag coefficients and then used as input for the CTF3 phase. The mag coefficients file can also be the output of the FFT3D. The CTF3 phase can be run using the mag coefficients file as input. The CTF3 phase can be run using the FFT3D generated MRC series as input.

Other.mag types

- For visualization otherwise maps (Pdbs-Fdbs) use pdbx.cif, fdbx.cif, fdbx.map, DensityMatcher to be added.
- For 3D Modeling, including composite print maps and iterative build and maps, use the Scipion plugins.
- Phantis also generate a simple simulated processing and map by selecting the interest point of the pdbx.cif file and using the PhenoCrystal with the mrc.preset.run.cif file is essentially the same as the Scipion simulated processing workflow.

List of all available keywords

```
ctf.fit = None
    path = None
    name = None

author = {}

protocol = None

ipix = None
jpix = None
ctf.defocus.range = 0,0
ctf.astig = None
ctf.phase.shift = None
ctf.cs.kev = None
ctf.mag
    pixelsize = None
    path = None
    name = None
    ctf.fit = None
    header = {}
    ctf.fit.path = None
    ctf.fit.name = FFT.log.mag

1.fdb.fdbp
    fdbp.path = None
    fdbp.name = None
    name = None
    mtx2fdbp.path = None

mtx2fdbp.path = None
mtx2fdbp.name = None
mtx2fdbp.cmd = None
mtx2fdbp.cmd.log = None

# FFT.log.mag.coefficients
# mtx2fdbp.cmd.log = mtx2fdbp -i mag -f fdb -spatial -fn map
# mtx2fdbp.cmd = mtx2fdbp -i mag -f fdb -spatial -pixelsize 1.0 -pixel
# mtx2fdbp.path = /home/phantis/.phantis/bin/mtx2fdbp
# mtx2fdbp.name = mtx2fdbp

# ctf.fit.path = /home/phantis/.phantis/bin/ctf.fit
# ctf.fit.name = ctf.fit

# header = {'Version': '20141', 'Nx': '4096', 'Ny': '4096', 'Nz': '1', 'Mode': '4', 'Nxstart': '0', 'Nystart': '0', 'Nzstart': '0', 'Mx': '4096', 'My': '4096', 'Mz': '1', 'Cell a': '4096.0', 'Cell b': '4096.0', 'Cell c': '1.0', 'Cell alpha': '90.0', 'Cell beta': '90.0', 'Cell gamma': '90.0', 'Mapc': '1', 'Mapr': '2', 'Maps': '3', 'Dmin': '-1.0', 'Dmax': '1.0', 'Dmean': '0.0', 'Ispg': '1', 'Nsymbt': '0', 'Extra': '', 'Exttyp': '', 'Nreal': '0', 'Nint': '0', 'Idtype': '0', 'Lens': '0', 'Nd1': '0', 'Nd2': '0', 'Vd1': '0', 'Vd2': '0', 'Tilt1': '0.0', 'Tilt2': '0.0', 'Tilt3': '0.0', 'Origin1': '0.0', 'Origin2': '0.0', 'Origin3': '0.0', 'Map': 'MAP', 'Machst': '68 68 0 0', 'Rms': '-1.0', 'Nlabl': '1', 'Label': 'mtx2fdbp -i mag -f fdb -spatial -pixelsize 1.0 -pixel -fn map'}

# header_keys = ['Version', 'Nx', 'Ny', 'Nz', 'Mode', 'Nxstart', 'Nystart', 'Nzstart', 'Mx', 'My', 'Mz', 'Cell a', 'Cell b', 'Cell c', 'Cell alpha', 'Cell beta', 'Cell gamma', 'Mapc', 'Mapr', 'Maps', 'Dmin', 'Dmax', 'Dmean', 'Ispg', 'Nsymbt', 'Extra', 'Exttyp', 'Nreal', 'Nint', 'Idtype', 'Lens', 'Nd1', 'Nd2', 'Vd1', 'Vd2', 'Tilt1', 'Tilt2', 'Tilt3', 'Origin1', 'Origin2', 'Origin3', 'Map', 'Machst', 'Rms', 'Nlabl', 'Label']

# header_values = ['20141', '4096', '4096', '1', '4', '0', '0', '0', '4096', '4096', '1', '4096.0', '4096.0', '1.0', '90.0', '90.0', '90.0', '1', '2', '3', '-1.0', '1.0', '0.0', '1', '0', '', '', '0', '0', '0', '0', '0', '0', '0.0', '0.0', '0.0', '0.0', '0.0', '0.0', 'MAP', '68 68 0 0', '-1.0', '1', 'mtx2fdbp -i mag -f fdb -spatial -pixelsize 1.0 -pixel -fn map']

# header_dimensions = [4096, 4096, 1]
# header_dimensions_defaults = [1, 1, 1]
# header_file_mode(int) = 4
# header_file_size = 67108864 (not used in compact ccp4)
```

multi_crystal_average

Phenix

Python based Hierarchical Environment for Integrated Crystallography

Density modification with multi-crystal averaging with phenix.multi_crystal_average

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Author(s)

- phenix.multi_crystal_average: Tom Terwilliger

Purpose

phenix.multi_crystal_average is a tool for carrying out density modification, including NCS symmetry within a crystal and solvent density from multiple crystals.

Usage

How phenix.multi_crystal_average works:

The inputs to phenix.multi_crystal_average are a set of PDB files that define the NCS within each crystal and the corresponding reflection data files. phenix.multi_crystal_average will find the NCS operators and the cross-crystal coefficients for each crystal, and carrying density-dependent maps for one or more crystals.

phenix.multi_crystal_average finds the NCS operators in each crystal using phenix.find_ncs_from_ncs_pdb and then uses the NCS operators and cross-crystal phase FOM files to construct replacement phases for each crystal. The cross-crystal phase FOM files are created using phenix.cross_crystal_phase_fom, which uses a set of NCS relationships and the NCS unit cell, and creates a score for a number of NCS operators for each pair of crystals. phenix.cross_crystal_phase_fom can be run separately if you want to specify the decisions for pairing from unique chain IDs, but you can use the default with phenix.go to do this for you. phenix.cross_crystal_phase_fom can also be used to determine which pairs of crystals are isomorphous (if there are more than one) or if the relationship from each chain pair should be modeled as a separate NCS group.

phenix.multi_crystal_average first uses the supplied PDB files to calculate NCS operators relating the NCS units within each crystal, and then uses the supplied cross-crystal phase FOM files to select a set of NCS operators for pairing the crystals. Finally, it uses these to carry out NCS averaging of the NCS relationships for each crystal, and carries out density-dependent map modification for one or more crystals. phenix.multi_crystal_average can be run with a set of crystal 1 phenix.refine output (average with composite phases) to make FOM files for each crystal to be used in the averaging, and can be run with phenix.refine output files for one or more crystals to carry out density-dependent averaging. If you request that the density-modified crystal 1 be refined, phenix.multi_crystal_average will carry out a set of phenix.refine cycles using the density-modified crystal 1 data and the original data for the other crystals. If the refined crystal 1 is then requested to be used in further averaging, phenix.multi_crystal_average will carry out a set of phenix.refine cycles using the density-modified crystal 1 data, with its output from the NCS averaging, the averaged set of phases for the other crystals, and the original data for the other crystals.

If the supplied PDB files have more than one domain or chain in each NCS asymmetric unit, then the domains or chains will be averaged in the NCS averaging.

Since NCS operators have been identified, density modification is carried out separately on data from each crystal, using the NCS operators and the corresponding cross-crystal phase information. phenix.multi_crystal_average also generates density maps for density modification or visualize the density map as NCS-related density is averaged. The density-modified maps are written out in CCP4 format.

For the expectation-and-SD NCS is defined, in this case including the density of all NCS copies within the crystal (the expectation) and the SD of the density in each NCS copy (the SD). The density-modified map is then the ratio of the density and when the NCS operators apply, it is expected to be equivalent to the SD scaled by an overall factor. phenix.multi_crystal_average can also carry out density-dependent averaging in which the density in each copy of the crystal is modified according to a map for the polymerized assembly is supplied by phenix.refine. phenix.multi_crystal_average can also carry out density-dependent averaging in which the density in each copy of the crystal is modified according to a map for the polymerized assembly is supplied by phenix.refine. In this case, the density-modified map is then the ratio of the density in each copy of the crystal to the density in the map. Alternatively, it can require that the density provided in your PDB file be used to define the NCS. If you specify that the density in your PDB file be used to define the NCS, then the density in each NCS group is limited to the region occupied by the corresponding chains in your PDB files.

phenix.multi_crystal_average can also be used to carry out density modification of crystal 1 copy in this crystal, the average density for all other NCS copies in this and other crystals is used as a target.

Finally, statistical density modification is carried out using histograms of expected density, solvent flattening, and flat solvent modification. Histogram matching is carried out using the histogram of the density in each crystal as the target. Solvent flattening and flat solvent modification are carried out using a solvent mask generated using phenix.mask and the corresponding solvent fraction. Solvent flattening is carried out using phenix.solve.

This entire process is carried out several times, looping to determine density maps for all crystals that typically converge in a few cycles of averaging (which will be faster if you provide a set of coordinates for corresponding NCS regions in different crystals).

Output files from phenix.multi_crystal_average

averaged_cycle_1_1.ccp4 Density-modified map coefficients for crystal 1, cycle 1. Crystal 1 is the first crystal specified, and cycle 1 is the first cycle of averaging.

density_mod_cycle_1_1.ccp4 Density-modified map coefficients for crystal 1, cycle 1. These map coefficients are the ratio of the density in the averaged map to the density in the NCS-related copies of the crystal. This is appropriate for a differences-based refinement of crystal 1 (the map is zero when the density is consistent with the NCS-related copies, and positive where the density is enhanced).

Graphical interface

The GUI is found in the "Tools" category of the main interface. The configuration tab contains a set of files for the cross-form:

Once the dialog is successfully filled in and an OK button is pressed, the job is submitted to the Python GUI launcher and a crystal form file is created. Alternatively, you can edit the resulting crystal form file and save it for later use.

Now you can run the job from the command:

```
phenix.multi_crystal_average run_with.eff
```

In the Advanced tab, there are options for specifying cross-crystal phase FOM files, coefficients for crystal 1, map coefficients and cross-crystal phase FOM files for other crystals, and the number of cycles of averaging for crystal 1 and the other crystals. The second crystal has no density-mod, has data for F1 and sigF1 and FOM and the coefficients for crystal1 (F_data, sigF_data and FOM_data), and has a cross-crystal phase FOM file for the cross-crystal phase FOM between crystal 1 and crystal 2 (FOM_1_2_crystal_2). The third crystal is similar to crystal 2.

Examples

Standard run of phenix.multi_crystal_average:

Running phenix.multi_crystal_average from the command line is easy. Usually you will want to add a crystal parameter file (run_with.eff) to contain your commands like this:

```
phenix.multi_crystal_average run_with.eff
# run_with.eff
crystal {
  name = native_1
  mtz = native_1.mtz
  pdb_in = native_1.pdb
  cross_crystal_phase_fom = cross_native_native_1.mtz
  # cross_crystal_phase_fom = CROSS_CRYSTAL_PHASE_FOM FOM_NATIVE_NATIVE_1 NATIVE_1 NATIVE
  # cycles = 1
}
crystal {
  name = native_2
  mtz = native_2.mtz
  pdb_in = native_2.pdb
  cross_crystal_phase_fom = cross_native_native_2.mtz
  cycles = 1
}
```

Then you can run the job from the command:

```
phenix.multi_crystal_average run_with.eff
```

In this example we have two crystals, "native_1" and "native_2" providing map coefficients in crystal 1, map coefficients and cross-crystal phase FOM files for other crystals, and the number of cycles of averaging for crystal 1 and the other crystals. The second crystal has no density-mod, has data for F2 and sigF2 and FOM and the coefficients for crystal1 (F_data, sigF_data and FOM_data), and has a cross-crystal phase FOM file for the cross-crystal phase FOM between crystal 1 and crystal 2 (FOM_1_2_crystal_2). The third crystal is similar to crystal 2.

In this example, the density-modified map coefficients are written out in CCP4 format, and phenix.refine can be used to carry out refinement using these coefficients, and you will want to supply hyperbolic weights and a differences-based target.

The crystal field stands for "Multi-crystal" and contains: if you are running "Run" from phenix.multi_crystal_average in the GUI, you will need to specify the name of the crystal, the mtz file, the pdb file, the cross_crystal_phase_fom, the FOM, the number of cycles, and the name of the output "cross_crystal_phase_fom" file. Only one cycle, one mtz, one pdb, one cross_crystal_phase_fom and one output "cross_crystal_phase_fom" file are allowed. Then enter a crystal name, the mtz file, the pdb file, and the cross_crystal_phase_fom file and press "Save to Crystal".

Run of phenix.multi_crystal_average with multiple domains:

If your PDB files have more than one NCS domain within a chain, then you may want to split the chains up into separate domains. phenix.multi_crystal_average will do this automatically if you specify the number of domains in the NCS group.

Here we run the PDB file 1ccd.pdb (2 in 2) by hand. The PDB 1ccd.pdb has one chain and contains dimers so the domains that are specific to "dimer_chains.def".

```
phenix.multi_crystal_average 1ccd.pdb dimer_chains.def
```

Now we have two domains per chain, and we need to have cross-crystal phase FOM files for each domain. In this example we have two crystals, "native_1" and "native_2" providing map coefficients in crystal 1, map coefficients and cross-crystal phase FOM files for other crystals, and the number of cycles of averaging for crystal 1 and the other crystals. The second crystal has no density-mod, has data for F2 and sigF2 and FOM and the coefficients for crystal1 (F_data, sigF_data and FOM_data), and has a cross-crystal phase FOM file for the cross-crystal phase FOM between crystal 1 and crystal 2 (FOM_1_2_crystal_2). The third crystal is similar to crystal 2.

In this example, the density-modified map coefficients are written out in CCP4 format, and phenix.refine can be used to carry out refinement using these coefficients, and you will want to supply hyperbolic weights and a differences-based target.

Run of phenix.multi_crystal_average with phenix.refine NCS automatic unit cell expansion:

If you have NCS relationships that are specified in phenix.refine format, then you may want to split the chains up into separate domains. phenix.multi_crystal_average will do this automatically if you specify the number of domains in the NCS group.

Here we run the PDB file 1ccd.pdb (2 in 2) by hand. The PDB 1ccd.pdb has one chain and contains dimers so the domains that are specific to "dimer_chains.def".

```
phenix.multi_crystal_average 1ccd.pdb dimer_chains.def
```

Now we have two domains per chain, and we need to have cross-crystal phase FOM files for each domain. In this example we have two crystals, "native_1" and "native_2" providing map coefficients in crystal 1, map coefficients and cross-crystal phase FOM files for other crystals, and the number of cycles of averaging for crystal 1 and the other crystals. The second crystal has no density-mod, has data for F2 and sigF2 and FOM and the coefficients for crystal1 (F_data, sigF_data and FOM_data), and has a cross-crystal phase FOM file for the cross-crystal phase FOM between crystal 1 and crystal 2 (FOM_1_2_crystal_2). The third crystal is similar to crystal 2.

In this example, the density-modified map coefficients are written out in CCP4 format, and phenix.refine can be used to carry out refinement using these coefficients, and you will want to supply hyperbolic weights and a differences-based target.

Using phenix.refine as a refiner:

phenix.multi_crystal_average can be used as a refiner (modifies one of crystals) and averaging with NCS as well as cross-averaging map coefficients, and you will want to supply hyperbolic weights and a differences-based target.

The crystal field stands for "Multi-crystal" and contains: if you are running "Run" from phenix.multi_crystal_average in the GUI, you will need to specify the name of the crystal, the mtz file, the pdb file, the cross_crystal_phase_fom, the FOM, the number of cycles, and the name of the output "cross_crystal_phase_fom" file. Only one cycle, one mtz, one pdb, one cross_crystal_phase_fom and one output "cross_crystal_phase_fom" file are allowed. Then enter a crystal name, the mtz file, the pdb file, and the cross_crystal_phase_fom file and press "Save to Crystal".

Output files:

Additional information:

Frequently asked questions

```
phenix.pdbtools GPR90CryoEM-cons-cryo-model-box.pdb chain ss "(1:L,2:M:9016,7:L:140
```

The file pdb_chain.pdb is expected should look like:

```
> 1:L
> 2:M:9016
> 7:L:140
> 8:L:
> 9:M:
> 10:M:
> 11:M:
> 12:M:
> 13:M:
> 14:M:
> 15:M:
> 16:M:
> 17:M:
> 18:M:
> 19:M:
> 20:M:
> 21:M:
> 22:M:
> 23:M:
> 24:M:
> 25:M:
> 26:M:
> 27:M:
> 28:M:
> 29:M:
> 30:M:
> 31:M:
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> 130:M:
> 131:M:
> 132:M:
> 133:M:
> 134:M:
> 135:M:
> 136:M:
> 137:M:
> 138:M:
> 139:M:
> 140:M:
```

where the letter and number stands for chain ID and residue range for a particular domain. You should specify the chain ID and the residue range for each domain.

Run of phenix.multi_crystal_average using PDB files to define the NCS asymmetric unit:

phenix.multi_crystal_average -d -n 0 -r -m 0.95 -p ncs_group_def=pdb_chain.pdb

Output: pdb_chain_ncs_ave_unit_cryo.pdb

Possible Problems

Specific limitations and problems:

- The current implementation of NCS averaging in phenix.multi_crystal_average (tested: Dmitri's list of PDB files) will not work if the NCS operators are not orthogonal.
- If the NCS asymmetric unit of your crystal contains more than one type of chain, phenix.multi_crystal_average requires that the order of chains in the NCS asymmetric unit in the pdb file (chain1, chain2, chain3, chain4) matches exactly the order of chains in the NCS asymmetric unit in the pdb file (chain1, chain2, chain3, chain4). Otherwise, phenix.multi_crystal_average will fail. If you would need to rename your chains and residues so that all the molecules in a single NCS group have the same chain and residue IDs, you can use phenix.pdbtools to do that. Alternatively, you can use the ncs_group_def=pdb_chain.pdb option to specify the chain and residue ranges for each NCS group. Please make sure that the chain IDs in the NCS asymmetric unit are unique.
- If your NCS asymmetric unit has more than one domain (more than one type of chain chain), or other non-protein chains (ligands, waters, etc), phenix.multi_crystal_average will fail unless you specify the chain IDs (chain1, chain2, chain3, chain4) that are to be averaged in the pdb file. This is because phenix.multi_crystal_average requires that the order of chains in the NCS asymmetric unit in the pdb file (chain1, chain2, chain3, chain4) matches exactly the order of chains in the NCS asymmetric unit in the pdb file (chain1, chain2, chain3, chain4). Alternatively, you can use the ncs_group_def=pdb_chain.pdb option to specify the chain and residue ranges for each NCS group. Please make sure that the chain IDs in the NCS asymmetric unit are unique.
- Normally you should supply PDB files defining the NCS in your crystal in which all the chains have the same chain and residue IDs. Alternatively, you can use the ncs_group_def=pdb_chain.pdb option to specify the chain and residue ranges for each NCS group. Please make sure that the chain IDs in the NCS asymmetric unit are unique.

```
ncs_group_def=pdb_chain.pdb
```

- The use of the asymmetric unit in the EQUIVALENCY section of phenix.multi_crystal_average is limited to the case when the NCS asymmetric unit is the same as the asymmetric unit of the crystal. Otherwise, phenix.multi_crystal_average will fail. Use phenix.ncs_ave_unit_cryo.pdb instead.

Literature

- **Rapid phenixRMSD NCS identification using heavy-atom substructures**, TC, Terwilliger, Acta Crystallogr D Struct Biol 75, 1-7 (2019)
- **Statistical density modification with non-crystallographic symmetry**, TC, Terwilliger, Acta Crystallogr D Struct Biol 57, 1755-1762 (2001)
- **Maximum-likelihood density modification**, TC, Terwilliger, Acta Crystallogr D Biol Crystallogr 56, 965-972 (2000)
- **Decision-theoretic phasing**, TC, Terwilliger, Acta Crystallogr A Found Crystallogr 57, 1763-75 (2001)

Additional information

List of all available keywords

```
phenix.multi_crystal_average d=True n=0 r=True m=0.95 ncs_ave_unit_cryo=True

crystal
  ncs_group_def = None
                  PDB file for identifying chains assigned to ncs groups. If specified,
                  ONLY the chains in the ncs_group_def will be averaged.
                  Use this if the ncs asymmetric unit is different from the
                  crystal asymmetric unit (EQUIVALENCY section of the output).
                  Note: chain IDs in the ncs_group_def file should be unique.
                  Note: if the ncs_group_def file has more than one chain, the
                  order of chains in the ncs_group_def file should match the
                  order of chains in the ncs asymmetric unit.
                  Note: if the ncs_group_def file has more than one chain,
                  all chain and res selections (ncs_ref=chain1 ncs_target=chain2
                  ncs_ref=chain3 ncs_target=chain4 ncs_ref=chain5 ncs_target=chain6
                  ncs_ref=chain7 ncs_target=chain8 ncs_ref=chain9 ncs_target=chain10)
                  will be ignored.
  ncs_ref = None
  ncs_target = None
  ncs_chain_id = None
  ncs_chain_id_ref = None
  ncs_chain_id_target = None
  ncs_ref_selection = None
  ncs_target_selection = None
  ncs_ref_selection_1 = None
  ncs_target_selection_1 = None
  ncs_ref_selection_2 = None
  ncs_target_selection_2 = None
  ncs_ref_selection_3 = None
  ncs_target_selection_3 = None
  ncs_ref_selection_4 = None
  ncs_target_selection_4 = None
  ncs_ref_selection_5 = None
  ncs_target_selection_5 = None
  ncs_ref_selection_6 = None
  ncs_target_selection_6 = None
```

Building biological assembly and crystallographic asymmetric unit from a PDB file

Introduction

In PDB files, all of the atoms belonging to a single molecule are in the crystallographic asymmetric unit of the unit cell. In such cases necessary information, contained and necessary for both crystallographic and non-crystallographic applications, such as the biological assembly and the crystallographic asymmetric unit, are lost.

Phenix provides commands to create a pdb file of the reconstructed or restored, for both the biological assembly and the crystallographic asymmetric unit.

Reconstruction of the biological assembly and crystallographic asymmetric unit from the pdb file RCSB000 (PDB ID 1ubq) is one of the cases, provided two chain sets are reconstructed and also there is no current information in the PDB file about the reconstruction. Use this case, using the RCSB data.

Command-line use

Biological Assembly

```
phenix.pdbtools molecular_reconstruction ipdf_file=1ubq.pdb
Keywords:
  verbose = True
  ncs = True

Fixed:
  ncs_phil_path=None
  ncs_file_name=None
  ncs_chain_limit=None
  ncs_copies_limit=None
  ncs_search_method=exhaustive
  ncs_search_resolution=None
  ncs_search_max_rms=None
  ncs_search_min_cc=None
  ncs_search_min_dist_factor=None
  ncs_search_max_dist_factor=None
  ncs_search_max_ncs_molecules_per_asu=None
  ncs_search_max_ncs_ncs_molecules=None
  ncs_search_max_ncs_asu_molecules=None
  ncs_search_chain_type=None
  ncs_search_output_dir=None
  ncs_search_output_prefix=None
  ncs_search_write_log=False
  ncs_search_write_pdb=False
  ncs_search_write_ncs_phil=False
  ncs_search_write_asu_pdb=False
  ncs_search_write_ncs_pdb=False
  ncs_search_write_ncs_asu_pdb=False
  ncs_search_write_ncs_ncs_pdb=False
  ncs_search_write_asu_asu_pdb=False
  ncs_search_write_ncs_asu_asu_pdb=False
  ncs_search_write_asu_ncs_asu_pdb=False
  ncs_search_write_ncs_ncs_ncs_pdb=False
  ncs_search_write_asu_ncs_ncs_pdb=False
  ncs_search_write_ncs_asu_ncs_pdb=False
  ncs_search_write_asu_asu_ncs_pdb=False
  ncs_search_write_ncs_ncs_asu_pdb=False
  ncs_search_write_asu_ncs_asu_pdb=False
  ncs_search_write_ncs_asu_asu_pdb=False
  ncs_search_write_asu_asu_asu_pdb=False
  ncs_search_write_ncs_ncs_ncs_ncs_pdb=False
  ncs_search_write_asu_ncs_ncs_ncs_pdb=False
  ncs_search_write_ncs_asu_ncs_ncs_pdb=False
  ncs_search_write_asu_asu_ncs_ncs_pdb=False
  ncs_search_write_ncs_ncs_asu_ncs_pdb=False
  ncs_search_write_asu_ncs_asu_ncs_pdb=False
  ncs_search_write_ncs_asu_asu_ncs_pdb=False
  ncs_search_write_asu_asu_asu_ncs_pdb=False
  ncs_search_write_ncs_ncs_ncs_asu_pdb=False
  ncs_search_write_asu_ncs_ncs_asu_pdb=False
  ncs_search_write_ncs_asu_ncs_asu_pdb=False
  ncs_search_write_asu_asu_ncs_asu_pdb=False
  ncs_search_write_ncs_ncs_asu_asu_pdb=False
  ncs_search_write_asu_ncs_asu_asu_pdb=False
  ncs_search_write_ncs_asu_asu_asu_pdb=False
  ncs_search_write_asu_asu_asu_asu_pdb=False
  ncs_search_write_ncs
```

Calculating a simple NCS averaged map

If you already have the asymmetric unit of the NCS operators, you can use phenix.map_symmetry and add ncs=ncs.ncs.spec to generate the NCS averaged map. Alternatively, you can use phenix.ncs_average to generate the NCS averaged map and also to find the NCS operators if they are not known.

The output of phenix.ncs_average is a CCP4 style map file.

These simple NCS and NCS masks can be also made from the ncsed with high NCS symmetry and they are useful for making NCS averaged maps and NCS masks for phenix.ncs_ccp4 and phenix.ncs_mask.

If you want to see the region that is being averaged, you can run phenix.ncs_average like this (notice the double quotes around the ncs_mask keyword):

```
phenix.ncs_average ncs_mask=PATH_TO_NCS_MASK PATH_TO_MAPS_FOR_AVERAGING OUT="ncs_mask.ccp4"
ncs_mask=ncs.ncs
```

This will write out the region to be averaged, you can do this by supplying a PDB file and the mask will be created using the PDB file. This can be very useful to check if there are any gaps in a chain trace around the NCS operators. Example of this is shown below:

```
phenix.ncs_average ncs_mask=PATH_TO_NCS_MASK PATH_TOMAPS_FOR_AVERAGING OUT="ncs_mask.ccp4"
ncs_mask=PATH_TO_PDB_FILE_FOR_MASK OUT="ncs_mask.ccp4"
```

List of all available keywords

```
input_files
  map_in .Map
    map_coeff_labels .Str                    input MTZ file with map coefficients
                                             A comma-separated pair of MTZ column labels, for example FWT,PHWT
                                             FWT,PHWT,DELFWT,PHDELFWT,FOM,HLA,HLB,HLC,HLD or FP,SIGFP,DANO,SIGDANO
                                             FP,SIGFP,FOM,HLA,HLB,HLC,HLD or FP,SIGFP,FOM,HLA,HLB,HLC,HLD or
                                             DEPOSIT,NATIVE,SIGNAT,NATIVE,FOM,PHNAT,HLANAT,HLBNAT,HLCNAT,HLDNAT
                                             DEPOSIT,DERIVATIVE,SIGNAT,DERIVATIVE,FOM,PHNAT,HLANAT,HLBNAT,HLCNAT,
                                             HLDNAT,DELFWT,PHDELWT,FOM or FP,SIGFP,DANO,SIGDANO,FOM,PHIB,HLA,HLB,
                                             HLC,HLD or FP,SIGFP,DANO,SIGDANO,FOM,PHIB,HLA,HLB,HLC,HLD or FP,
                                             SIGFP,DANO,SIGDANO,FOM,PHIB,HLA,HLB,HLC,HLD
    map_file .Path                           Map file
    ccp4_flag .Bool                          Flag to indicate that the file is in CCP4 format if map file
                                             ends with .map
    mtz_flag .Bool                           Flag to indicate that the file is in MTZ format if map file
                                             ends with .mtz, .hkl, .sca, .cns, .ccp4, .mtzmap, .mtz.gz,
                                             .hkl.gz, .sca.gz, .cns.gz, .ccp4.gz, .mtzmap.gz, .hkl.bz2,
                                             .sca.bz2, .cns.bz2, .ccp4.bz2, .mtzmap.bz2, .mtz.bz2, .hkl.Z,
                                             .sca.Z, .cns.Z, .ccp4.Z, .mtzmap.Z, .mtz.Z, .hkl.zip, .sca.zip,
                                             .cns.zip, .ccp4.zip, .mtzmap.zip, .mtz.zip, .hkl.tar, .sca.tar,
                                             .cns.tar, .ccp4.tar, .mtzmap.tar, .mtz.tar, .hkl.tar.gz,
                                             .sca.tar.gz, .cns.tar.gz, .ccp4.tar.gz, .mtzmap.tar.gz,
                                             .mtz.tar.gz, .hkl.tar.bz2, .sca.tar.bz2, .cns.tar.bz2,
                                             .ccp4.tar.bz2, .mtzmap.tar.bz2, .mtz.tar.bz2, .hkl.tar.Z,
                                             .sca.tar.Z, .cns.tar.Z, .ccp4.tar.Z, .mtzmap.tar.Z, .mtz.tar.Z,
                                             .hkl.tar.zip, .sca.tar.zip, .cns.tar.zip, .ccp4.tar.zip,
                                             .mtzmap.tar.zip, .mtz.tar.zip or .pdb
    pdb_file .Path
    pdb_labels .Str,optional,default=None    Select CRYS-records map file with multi-managed density
    ncs_spec .Ncs                            Input NCS information (.ncs_spec format)
    ncs_info_file .Path,optional             Output NCS information (.ncs_spec format)
    ncs_mask .Ncs                            Optional NCS mask (.ncs_spec format) to be used for masking
                                             the NCS averaged map
    ncs_mask_file_name .Path                 Optional PDB file to be used for masking. Note: if ncs_mask
                                             is not specified and this is set, NCS mask will be made from
                                             this file.
    ncs_file .Path                           NCS file (.ncs)
    output_file .Path,optional,default=ncs_  Filename for the output map averaging
  directories
    work_dir .Path,default=.                 Optional temporary work directory
    output_dir .Path,default=.               Output directory where files are to be written
  crystal_info
    resolution .Real                         High-resolution limit for map calculation
    sites_cart .Sites                        Atomic fractions
    unit_cell .UnitCell                      Unit cell parameters (Angstroms or fractional fractions)
    ucn_mod_id_ph_min .Int(>=0)              Min mod_id for ncs to be used for cell reparameterization
    ncs_type .Str                            Type of NCS (cartesian, rotation, or rotation-translation)
    high_resolution_limit .Real              Resolution at which map starts to be high-resolution system
                                             (resolution at which map starts to be high-resolution system
                                             for calculation of mask and FFT of high-resolution is done
                                             separately from low-resolution system)
    fraction_ncs_mask .Real                  Fraction of the unit cell volume occupied by NCS mask (used
                                             for memory allocation)
    solvent_fraction_parameters .Choice      Solvent fraction parameters
  ncs
    ncs_type .Choice                         Rotation center
      rotation .Choice                       Rotate about a point
        rotation_center_frac .Sites          Rotation center
      shift .Bool                            Shift along a set of directions
      rotation_shift .Bool                   Rotation and shift
    rotation_center_frac .Sites              Rotation center
  output
    output_ncs_file .Bool                    Optional output
      ncs_file_name .Path                    Output NCS file name
    output_ncs_mask .Bool                    Optional output NCS mask
      ncs_mask_file_name .Path               Output NCS mask file name
    output_map_file_name .Path               Output map file name
    output_mtz_parameters .Choice            Output MTZ parameters
      mtz_parameters
        output_mtz_file_name .Path           Optional temporary mtz directory
        output_dir .Path                     Output directory where files are to be written
  crystal_info
    resolution .Real                         High-resolution limit for map calculation
    solvent_content .Real                    Solvent fraction
    sites_cart .Sites                        Atomic fractions
    unit_cell .UnitCell                      Unit cell parameters (Angstroms or fractional fractions)
    ucn_mod_id_ph_min .Int(>=0)              Min mod_id for ncs to be used for cell reparameterization
    ncs_type .Str                            Type of NCS (cartesian, rotation, or rotation-translation)
    high_resolution_limit .Real              Resolution at which map starts to be high-resolution system
                                             (resolution at which map starts to be high-resolution system
                                             for calculation of mask and FFT of high-resolution is done
                                             separately from low-resolution system)
    fraction_ncs_mask .Real                  Fraction of the unit cell volume occupied by NCS mask (used
                                             for memory allocation)
    solvent_fraction_parameters .Choice      Solvent fraction parameters
  ncs
    ncs_type .Choice                         Rotation center
      rotation .Choice                       Rotate about a point
        rotation_center_frac .Sites          Rotation center
      shift .Bool                            Shift along a set of directions
      rotation_shift .Bool                   Rotation and shift
    rotation_center_frac .Sites              Rotation center
  output_ncs_mask .Bool                      Use ncs mask as the output average map
    ncs_mask_file_name .Path                 Use ncs mask as the output average map NOTE: if output_ncs_mask
                                             and ncs_mask_file_name are specified, ncs mask will be used as
                                             the output average map. If only output_ncs_mask is specified,
                                             output average map will be written out to the file
                                             "average_map_with_ncs_mask.ccp4" by default
```

Phenix *Python-based Hierarchical Environment for Integrated Xtallography*

Building starting with a very poor map with parallel_autobuild

Authors

parallel_autobuild: Tom Terwilliger

Purpose

The goal of parallel_autobuild is to build models starting from very poor maps. In the situation most of the model is incorrect and the map is very poor, it is necessary to make many changes to the model in order to improve the map and to improve the model.

The strategy implemented in parallel_autobuild is to find the regions of the density map in the neighborhood of the good the best model will fit. The strategy is then to carve a starting map and data, get the best model from this starting map, and then carve a new map and data centered on the best model and repeat the process. Starting the process may fields work to starting map that is good enough to yield a complete model.

How parallel autobuild works

Parallel_autobuild works by carving out a small density and creating a model from it. Parallel_autobuild runs automatically in a set of directories called parallel_autobuild_run_1, parallel_autobuild_run_2, parallel_autobuild_run_3, and so on. Each run of parallel_autobuild carves out a different region of the density and the corresponding map.

The choice of what is the best model is not always obvious. Parallel_autobuild uses the R values of the models to decide which is the best model. Parallel_autobuild also uses the R values of the models to decide which is the best model to be carved and rebuilt to make the choice.

Inputs for parallel autobuild

The inputs to parallel autobuild are the same as for autobuild, with the addition of a few control parameters. Parallel_autobuild can be run with a single set of inputs, or it can be run with a set of inputs specifying a list of the number of processors to use, the number of parallel runs, and the number of parallel autobuild jobs to be carved out. Parallel_autobuild can be run on a single processor, on a multiprocessor machine (e.g. with OpenMP), and on a set of machines (e.g. with MPI).

Parallel_autobuild can be run in a mode identical to that such as for the main line cycle has defined. If you supply a starting model the model obtained each cycle is used, and if you do not, it is based only into the last cycle.

It can, parallel-beyond phenix you to specify how jobs are to be run. Phenix autobuild can do run on a multiprocessor machine (e.g. with OpenMP) and such as parallel on a multiprocessor machine (e.g. with MPI).

Possible Problems

There may be no parallel autobuild the case where the map is very poor. MPI file and a map have opening for MPI OpenMP mode. Eg. Concurrent way to create the right file to run where autobuild with your data (you don't need to run the job, just the setup of the directories and files). Create Regions or create new other. Step into it needed to run data file for parallel autobuild.

PDB_XML_VERSION_MINOR

Minor version of the mmcif ontology used from different pdbx kits. It is possible that the use of pdbx_version_minor values indicates deprecated keyword definitions.

References:

Bioinformatics and Biology Insights: structure refinement and density modification with the PHENIX software suite [1] Thomas N. Pornillos, Oleg V. Sobolev, Pavel V. Afonine, Paul D. Adams, R. Bryan Sutton, Tom Alber, and Tom Terwilliger. doi:10.4137/BBI.S37099

Keywords:

List of all available keywords

_accession
_accession.date 1994-05-27 PRODELL: set code in compact file
_audit_conform
_audit_conform.dictionary Text name of conformance dictionary
_audit_conform.dict_location URL for a file or directory or machine resolvable service to access a copy of the dictionary against which the data block is to be checked for conformance. Use the CIF extension to the URL to indicate the MIME or compression type of the file.
_audit_conform.dict_name Name of conformance dictionary
_audit_conform.dict_version Version number of conformance dictionary. Text to follow the rules for a CIF data name, e.g. 1.0 or 1.0.3 or 1.0.3.alpha
_audit_creation_method
_audit_creation_method Software used for generation
_audit_creation_time
_audit_creation_time.date Date and time of creation
_audit_dictionary
_audit_dictionary.name Recognized dictionary name
_audit_dictionary.ver Best dictionary for mmCIF, PDBX/mmCIF,DDL/mmCIF,DDL1
_audit_editing_history
_audit_editing_history.date Date of editing session. Use the ISO standard format.
_audit_editing_history.text Free text description of the changes made in this editing session
_audit_update_record
_audit_update_record.date Date of update. Use the ISO standard format.
_audit_update_record.type Type of update
_audit_version
_audit_version.major Major version number
_audit_version.minor Minor version number
_audit_version.revision Revision version number
_axis
_axis.id Unique identifier for axis
_axis.type Type of axis
_axis_angle
_axis_angle.id Unique identifier for axis_angle
_axis_angle.angle_1 Angle to rotate about first axis
_axis_angle.angle_2 Angle to rotate about second axis
_axis_angle.angle_3 Angle to rotate about third axis
_axis_angle_esd
_axis_angle_esd.id Unique identifier for axis_angle_esd
_axis_angle_esd.angle_1_esd Estimated standard deviation for axis_angle.angle_1
_axis_angle_esd.angle_2_esd Estimated standard deviation for axis_angle.angle_2
_axis_angle_esd.angle_3_esd Estimated standard deviation for axis_angle.angle_3
_axis_angle_esd_ref
_axis_angle_esd_ref.id Unique identifier for axis_angle_esd_ref
_axis_angle_esd_ref.angle_1_esd_ref Reference for axis_angle_esd.angle_1_esd
_axis_angle_esd_ref.angle_2_esd_ref Reference for axis_angle_esd.angle_2_esd
_axis_angle_esd_ref.angle_3_esd_ref Reference for axis_angle_esd.angle_3_esd
_axis_ref
_axis_ref.id Unique identifier for axis_ref
_axis_ref.ref Reference for axis
_axis_type
_axis_type.id Unique identifier for axis_type
_axis_type.convention Convention for axis_type. Enumerated values are: 'CCP4' Axis type is defined by the CCP4 convention. 'PDB' Axis type is defined by the PDB convention.
_axis_type.detail Any additional information about axis_type
_axis_type_esd
_axis_type_esd.id Unique identifier for axis_type_esd
_axis_type_esd.convention_esd Estimated standard deviation for axis_type.convention
_axis_type_esd_ref
_axis_type_esd_ref.id Unique identifier for axis_type_esd_ref
_axis_type_esd_ref.convention_esd_ref Reference for axis_type_esd.convention_esd
_axis_type_ref
_axis_type_ref.id Unique identifier for axis_type_ref
_axis_type_ref.ref Reference for axis_type
_axis_unit_cell
_axis_unit_cell.id Unique identifier for axis_unit_cell
_axis_unit_cell.length_a_unit Unit of length_a
_axis_unit_cell.length_b_unit Unit of length_b
_axis_unit_cell.length_c_unit Unit of length_c
_axis_unit_cell.angle_alpha_unit Unit of angle_alpha
_axis_unit_cell.angle_beta_unit Unit of angle_beta
_axis_unit_cell.angle_gamma_unit Unit of angle_gamma
_axis_unit_cell_esd
_axis_unit_cell_esd.id Unique identifier for axis_unit_cell_esd
_axis_unit_cell_esd.length_a_unit_esd Estimated standard deviation for axis_unit_cell.length_a_unit
_axis_unit_cell.length_b_unit_esd Estimated standard deviation for axis_unit_cell.length_b_unit
_axis_unit_cell.length_c_unit_esd Estimated standard deviation for axis_unit_cell.length_c_unit
_axis_unit_cell.angle_alpha_unit_esd Estimated standard deviation for axis_unit_cell.angle_alpha_unit
_axis_unit_cell.angle_beta_unit_esd Estimated standard deviation for axis_unit_cell.angle_beta_unit
_axis_unit_cell.angle_gamma_unit_esd Estimated standard deviation for axis_unit_cell.angle_gamma_unit
_axis_unit_cell_esd_ref
_axis_unit_cell_esd_ref.id Unique identifier for axis_unit_cell_esd_ref
_axis_unit_cell_esd_ref.length_a_unit_esd_ref Reference for axis_unit_cell_esd.length_a_unit_esd
_axis_unit_cell_esd_ref.length_b_unit_esd_ref Reference for axis_unit_cell_esd.length_b_unit_esd
_axis_unit_cell_esd_ref.length_c_unit_esd_ref Reference for axis_unit_cell_esd.length_c_unit_esd
_axis_unit_cell_esd_ref.angle_alpha_unit_esd_ref Reference for axis_unit_cell_esd.angle_alpha_unit_esd
_axis_unit_cell_esd_ref.angle_beta_unit_esd_ref Reference for axis_unit_cell_esd.angle_beta_unit_esd
_axis_unit_cell_esd_ref.angle_gamma_unit_esd_ref Reference for axis_unit_cell_esd.angle_gamma_unit_esd
_axis_unit_cell_ref
_axis_unit_cell_ref.id Unique identifier for axis_unit_cell_ref
_axis_unit_cell_ref.length_a_unit_ref Reference for axis_unit_cell.length_a_unit
_axis_unit_cell_ref.length_b_unit_ref Reference for axis_unit_cell.length_b_unit
_axis_unit_cell_ref.length_c_unit_ref Reference for axis_unit_cell.length_c_unit
_axis_unit_cell_ref.angle_alpha_unit_ref Reference for axis_unit_cell.angle_alpha_unit
_axis_unit_cell_ref.angle_beta_unit_ref Reference for axis_unit_cell.angle_beta_unit
_axis_unit_cell_ref.angle_gamma_unit_ref Reference for axis_unit_cell.angle_gamma_unit
_axis_vector
_axis_vector.id Unique identifier for axis_vector
_axis_vector.x Component of axis_vector along the x axis
_axis_vector.y Component of axis_vector along the y axis
_axis_vector.z Component of axis_vector along the z axis
_axis_vector_esd
_axis_vector_esd.id Unique identifier for axis_vector_esd
_axis_vector_esd.x_esd Estimated standard deviation for axis_vector.x
_axis_vector_esd.y_esd Estimated standard deviation for axis_vector.y
_axis_vector_esd.z_esd Estimated standard deviation for axis_vector.z
_axis_vector_esd_ref
_axis_vector_esd_ref.id Unique identifier for axis_vector_esd_ref
_axis_vector_esd_ref.x_esd_ref Reference for axis_vector_esd.x_esd
_axis_vector_esd_ref.y_esd_ref Reference for axis_vector_esd.y_esd
_axis_vector_esd_ref.z_esd_ref Reference for axis_vector_esd.z_esd
_axis_vector_ref
_axis_vector_ref.id Unique identifier for axis_vector_ref
_axis_vector_ref.ref Reference for axis_vector
_cell
_cell.entry_id Unique identifier for a set of cell parameters
_cell.length_a Length of the unit cell a
_cell.length_b Length of the unit cell b
_cell.length_c Length of the unit cell c
_cell.angle_alpha Angle of the unit cell alpha
_cell.angle_beta Angle of the unit cell beta
_cell.angle_gamma Angle of the unit cell gamma
_cell.volume Volume of the unit cell
_cell.Z_PDB Number of the unit cell formulas in the PDB entry
_cell.pdbx_unique_axis Unique axis for monoclinic cell setting. Enumerated values are: 'a' Unique axis is a. 'b' Unique axis is b. 'c' Unique axis is c.
_cell_measurement
_cell_measurement.entry_id Unique identifier for a set of cell measurements
_cell_measurement.method Method used to measure the cell parameters
_cell_measurement.date_begin Date when measurement of cell parameters began. Use the ISO standard format.
_cell_measurement.date_end Date when measurement of cell parameters ended. Use the ISO standard format.
_cell_measurement.pressure Pressure in kilopascals at which the cell parameters were measured
_cell_measurement.pressure_esd Estimated standard deviation of cell_measurement.pressure
_cell_measurement.pressure_gradient Pressure gradient in megapascals per millimetre
_cell_measurement.temperature Temperature in kelvins at which the cell parameters were measured
_cell_measurement.temperature_esd Estimated standard deviation of cell_measurement.temperature
_cell_measurement.temperature_gradient Temperature gradient in kelvins per millimetre
_cell_measurement_refln
_cell_measurement_refln.crystal_id Unique identifier for a set of crystals
_cell_measurement_refln.wavelength_id Unique identifier for a set of wavelengths
_cell_measurement_refln.scan_id Unique identifier for a set of scan parameters
_cell_measurement_refln.ccd_id Unique identifier for a set of CCD parameters
_cell_measurement_refln.refln_id Unique identifier for a set of reflections
_cell_measurement_refln_ref
_cell_measurement_refln_ref.crystal_id Reference for cell_measurement_refln.crystal_id
_cell_measurement_refln_ref.wavelength_id Reference for cell_measurement_refln.wavelength_id
_cell_measurement_refln_ref.scan_id Reference for cell_measurement_refln.scan_id
_cell_measurement_refln_ref.ccd_id Reference for cell_measurement_refln.ccd_id
_cell_measurement_refln_ref.refln_id Reference for cell_measurement_refln.refln_id
_cell_measurement_ref
_cell_measurement_ref.entry_id Reference for cell_measurement.entry_id
_cell_measurement_target
_cell_measurement_target.entry_id Reference for cell_measurement.entry_id
_cell_reduced
_cell_reduced.entry_id Unique identifier for a set of reduced cell parameters
_cell_reduced.length_a Length of the reduced unit cell a
_cell_reduced.length_b Length of the reduced unit cell b
_cell_reduced.length_c Length of the reduced unit cell c
_cell_reduced.angle_alpha Angle of the reduced unit cell alpha
_cell_reduced.angle_beta Angle of the reduced unit cell beta
_cell_reduced.angle_gamma Angle of the reduced unit cell gamma
_cell_reduced.volume Volume of the reduced unit cell
_cell_reduced_ref
_cell_reduced_ref.entry_id Reference for cell_reduced.entry_id
_cell_setting
_cell_setting.entry_id Unique identifier for a set of cell settings
_cell_setting.type Type of cell setting
_chemical_conn_atom
_chemical_conn_atom.id Unique identifier for chemical_conn_atom
_chemical_conn_atom.type_id Type of atom
_chemical_conn_atom.charge Formal charge of atom
_chemical_conn_bond
_chemical_conn_bond.id Unique identifier for chemical_conn_bond
_chemical_conn_bond.type_id Type of bond
_chemical_formula
_chemical_formula.id Unique identifier for chemical_formula
_chemical_formula.type Type of chemical formula
_chemical_formula.weight Formula weight
_chemical_formula_atom
_chemical_formula_atom.id Unique identifier for chemical_formula_atom
_chemical_formula_atom.type_id Type of atom
_chemical_formula_atom.number Number of atoms
_chemical_formula_esd
_chemical_formula_esd.id Unique identifier for chemical_formula_esd
_chemical_formula_esd.weight_esd Estimated standard deviation for chemical_formula.weight
_chemical_formula_esd_ref
_chemical_formula_esd_ref.id Reference for chemical_formula_esd.id
_chemical_formula_esd_ref.weight_esd_ref Reference for chemical_formula_esd.weight_esd
_chemical_formula_ref
_chemical_formula_ref.id Reference for chemical_formula.id
_chemical_formula_type
_chemical_formula_type.id Unique identifier for chemical_formula_type
_chemical_formula_type.primary Indicates if this formula is the primary formula. Enumerated values are: 'yes' This formula is the primary formula. 'no' This formula is not the primary formula.
_chemical_formula_weight_atom_nuclide
_chemical_formula_weight_atom_nuclide.id Unique identifier for chemical_formula_weight_atom_nuclide
_chemical_formula_weight_atom_nuclide.atom_id Atom
_chemical_formula_weight_atom_nuclide.mass_number Mass number of nuclide
_chemical_formula_weight_atom_nuclide.weight Formula weight
_chemical_formula_weight_esd
_chemical_formula_weight_esd.id Unique identifier for chemical_formula_weight_esd
_chemical_formula_weight_esd.weight_esd Estimated standard deviation for chemical_formula_weight.weight
_chemical_formula_weight_esd_ref
_chemical_formula_weight_esd_ref.id Reference for chemical_formula_weight_esd.id
_chemical_formula_weight_esd_ref.weight_esd_ref Reference for chemical_formula_weight_esd.weight_esd
_chemical_formula_weight_ref
_chemical_formula_weight_ref.id Reference for chemical_formula_weight.id
_chemical_formula_weight_type
_chemical_formula_weight_type.id Unique identifier for chemical_formula_weight_type
_chemical_formula_weight_type.primary Indicates if this formula weight is the primary formula weight. Enumerated values are: 'yes' This formula weight is the primary formula weight. 'no' This formula weight is not the primary formula weight.
_chemical_oxidation_number
_chemical_oxidation_number.id Unique identifier for chemical_oxidation_number
_chemical_oxidation_number.atom_id Atom
_chemical_oxidation_number.oxidation_number Oxidation number
_chemical_oxidation_number_esd
_chemical_oxidation_number_esd.id Unique identifier for chemical_oxidation_number_esd
_chemical_oxidation_number_esd.oxidation_number_esd Estimated standard deviation for chemical_oxidation_number.oxidation_number
_chemical_oxidation_number_esd_ref
_chemical_oxidation_number_esd_ref.id Reference for chemical_oxidation_number_esd.id
_chemical_oxidation_number_esd_ref.oxidation_number_esd_ref Reference for chemical_oxidation_number_esd.oxidation_number_esd
_chemical_oxidation_number_ref
_chemical_oxidation_number_ref.id Reference for chemical_oxidation_number.id
_chemical_oxidation_number_type
_chemical_oxidation_number_type.id Unique identifier for chemical_oxidation_number_type
_chemical_oxidation_number_type.primary Indicates if this oxidation number is the primary oxidation number. Enumerated values are: 'yes' This oxidation number is the primary oxidation number. 'no' This oxidation number is not the primary oxidation number.
_chemical_properties_biological
_chemical_properties_biological.entry_id Unique identifier for a set of biological properties
_chemical_properties_biological.blood_coagulation Blood coagulation properties
_chemical_properties_biological.blood_flow Blood flow properties
_chemical_properties_biological.biological_activity Biological activity
_chemical_properties_biological.biological_detail Any additional information about biological properties
_chemical_properties_biological_ref
_chemical_properties_biological_ref.entry_id Reference for chemical_properties_biological.entry_id
_chemical_properties_chemical
_chemical_properties_chemical.entry_id Unique identifier for a set of chemical properties
_chemical_properties_chemical.melting_point Melting point
_chemical_properties_chemical.melting_point_gradient Melting point gradient in megapascals per millimetre
_chemical_properties_chemical.melting_point_range Melting point range
_chemical_properties_chemical.optical_activity Optical activity
_chemical_properties_chemical.solubility Solubility
_chemical_properties_chemical.solubility_detail Any additional information about solubility
_chemical_properties_chemical.solubility_product Solubility product
_chemical_properties_chemical.solubility_product_temperature Temperature at which the solubility product was measured
_chemical_properties_chemical.solubility_product_pH pH at which the solubility product was measured
_chemical_properties_chemical.solubility_product_pH_range pH range at which the solubility product was measured
_chemical_properties_chemical.solubility_product_pH_detail Any additional information about the pH at which the solubility product was measured
_chemical_properties_chemical_ref
_chemical_properties_chemical_ref.entry_id Reference for chemical_properties_chemical.entry_id
_chemical_properties_crystal
_chemical_properties_crystal.entry_id Unique identifier for a set of crystal properties
_chemical_properties_crystal.color Color of crystals
_chemical_properties_crystal.hardness Hardness of crystals
_chemical_properties_crystal.smell Smell of crystals
_chemical_properties_crystal.solubility Solubility of crystals
_chemical_properties_crystal.solubility_detail Any additional information about solubility of crystals
_chemical_properties_crystal_ref
_chemical_properties_crystal_ref.entry_id Reference for chemical_properties_crystal.entry_id
_chemical_properties_physical
_chemical_properties_physical.entry_id Unique identifier for a set of physical properties
_chemical_properties_physical.absorption Absorption properties
_chemical_properties_physical.absorption_detail Any additional information about absorption properties
_chemical_properties_physical.color Color
_chemical_properties_physical.dielectric_constant Dielectric constant
_chemical_properties_physical.dielectric_constant_detail Any additional information about dielectric constant
_chemical_properties_physical.dielectric_constant_temperature Temperature at which the dielectric constant was measured
_chemical_properties_physical.dielectric_constant_pH pH at which the dielectric constant was measured
_chemical_properties_physical.dielectric_constant_pH_range pH range at which the dielectric constant was measured
_chemical_properties_physical.dielectric_constant_pH_detail Any additional information about the pH at which the dielectric constant was measured
_chemical_properties_physical.density Density
_chemical_properties_physical.density_Mathews Density according to Mathews
_chemical_properties_physical.density_Mathews_detail Any additional information about density according to Mathews
_chemical_properties_physical.density_measured Measured density
_chemical_properties_physical.density_measured_detail Any additional information about measured density
_chemical_properties_physical.density_measured_temperature Temperature at which the density was measured
_chemical_properties_physical.density_measured_pH pH at which the density was measured
_chemical_properties_physical.density_measured_pH_range pH range at which the density was measured
_chemical_properties_physical.density_measured_pH_detail Any additional information about the pH at which the density was measured
_chemical_properties_physical.density_measured_pressure Pressure at which the density was measured
_chemical_properties_physical.density_measured_pressure_detail Any additional information about the pressure at which the density was measured
_chemical_properties_physical.density_measured_pressure_method Method used to measure the pressure at which the density was measured
_chemical_properties_physical.density_measured_pressure_range Pressure range at which the density was measured
_chemical_properties_physical.density_measured_temperature_range Temperature range at which the density was measured
_chemical_properties_physical.density_measured_temperature_method Method used to measure the temperature at which the density was measured
_chemical_properties_physical.density_measured_temperature_detail Any additional information about the temperature

auto_vehicle_lock	Type: Boolean Default: false Vehicle will lock when it is locked, the app will lock the vehicle shortly after you walk away from the vehicle.
auto_vehicle_unlock	Type: Boolean Default: false Vehicle will unlock when you approach with your key.
auto_tonneau_open_speed	Type: Integer Range: 0 to 100 Unit: km/h Default: 0 Tonneau will open if the vehicle speed exceeds the specified threshold. Setting this value to 0 disables the feature.
auto_tonneau_close_speed	Type: Integer Range: 0 to 100 Unit: km/h Default: 0 Tonneau will close if the vehicle speed exceeds the specified threshold. Setting this value to 0 disables the feature.
auto_tonneau_close_offset	Type: Integer Range: 0 to 100 Unit: km/h Default: 0 Tonneau will close if the vehicle speed exceeds the specified threshold minus the offset. Setting this value to 0 disables the feature.
auto_tonneau_close_timeout	Type: Integer Range: 0 to 300 Unit: seconds Default: 0 Tonneau will close after the specified timeout if the vehicle speed is below the specified threshold. Setting this value to 0 disables the feature.
auto_tonneau_close_lock	Type: Boolean Default: false Tonneau will close and lock if the vehicle is locked.
vehicle_alerts	
alert_max_distance_from_home	Type: Integer Range: 0 to 1000 Unit: km Default: 0 Alert if vehicle is more than the specified distance from home. Setting this value to 0 disables the feature.
alert_max_duration	Type: Integer Range: 0 to 1440 Unit: minutes Default: 0 Alert if vehicle is not parked for longer than the specified duration. Setting this value to 0 disables the feature.
alert_service_duration	Type: Integer Range: 0 to 1440 Unit: minutes Default: 0 Alert if vehicle is in service for longer than the specified duration. Setting this value to 0 disables the feature.
alert_service_visit	Type: Boolean Default: false Alert if vehicle is in service.
charging	
charge_limit_soc	Type: Integer Range: 50 to 100 Unit: % Default: 90 Set the charge limit state of charge (SoC) to the specified value. Setting this value to 100 disables the charge limit.
charge_limit_soc_std	Type: Integer Range: 50 to 100 Unit: % Default: 90 Set the charge limit state of charge (SoC) to the specified value for standard charging.
charge_limit_soc_max	Type: Integer Range: 50 to 100 Unit: % Default: 90 Set the charge limit state of charge (SoC) to the specified value for maximum charging.
charge_amps	Type: Integer Range: 5 to 32 Unit: A Default: 32 Set the charge current to the specified value.
charge_location	Type: Integer Range: -32768 to 32767 Default: 0 Set the charge location to the specified value.
charge_latitude	Type: Integer Range: -32768 to 32767 Default: 0 Set the charge latitude to the specified value.
charge_longitude	Type: Integer Range: -32768 to 32767 Default: 0 Set the charge longitude to the specified value.
charge_schedule_enabled	Type: Boolean Default: false Enable charge schedule.
charge_schedule_data	Type: Blob Max length: 65535 Charge schedule data.
preconditioning_enabled	Type: Boolean Default: false Enable preconditioning.
preconditioning_times	Type: Enumeration Allowed values: all_week, weekdays, weekends Default: all_week Set the preconditioning times to the specified value.
preconditioning_schedule_data	Type: Blob Max length: 65535 Preconditioning schedule data.
scheduled_charging_mode	Type: Enumeration Allowed values: off, depart, all_week, weekdays, weekends Default: off Set the scheduled charging mode to the specified value.
scheduled_charging_time	Type: Integer Range: 0 to 1440 Unit: minutes Default: 0 Set the scheduled charging time to the specified value.
charge_port_door_open	Type: Boolean Default: false Open the charge port door.
charge_port_latch	Type: Enumeration Allowed values: engaged, blank, unpowered Default: engaged Set the charge port latch to the specified value.
charge_to_max_range	Type: Boolean Default: false Set the charge limit to the maximum range.
climate	
climate_keeper_mode	Type: Enumeration Allowed values: off, on, dog, camp Default: off Set the climate keeper mode to the specified value.
cabin_overheat_protection	Type: Boolean Default: false Enable cabin overheat protection.
cabin_overheat_protection_temperature	Type: Enumeration Allowed values: 40_C, 35_C, 30_C Default: 40_C Set the cabin overheat protection temperature to the specified value.
cabin_overheat_protection_actively_cooling	Type: Boolean Default: false Enable cabin overheat protection actively cooling.
allow_cabin_overheat_protection	Type: Boolean Default: false Allow cabin overheat protection.
hvac_auto	Type: Boolean Default: false Set the HVAC auto to the specified value.
hvac_power	Type: Boolean Default: false Set the HVAC power to the specified value.
hvac_fan_speed	Type: Integer Range: 0 to 100 Unit: % Default: 0 Set the HVAC fan speed to the specified value.
hvac_fan_status	Type: Integer Range: 0 to 100 Default: 0 Set the HVAC fan status to the specified value.
hvac_temperature_units	Type: Enumeration Allowed values: F, C Default: F Set the HVAC temperature units to the specified value.
hvac_left_temperature_request	Type: Integer Range: -32768 to 32767 Default: 0 Set the HVAC left temperature request to the specified value.
hvac_right_temperature_request	Type: Integer Range: -32768 to 32767 Default: 0 Set the HVAC right temperature request to the specified value.
hvac_seat_cooler_left	Type: Enumeration Allowed values: unknown, off, low, high Default: unknown Set the HVAC seat cooler left to the specified value.
hvac_seat_cooler_right	Type: Enumeration Allowed values: unknown, off, low, high Default: unknown Set the HVAC seat cooler right to the specified value.
hvac_seat_heater_left	Type: Integer Range: 0 to 3 Default: 0 Set the HVAC seat heater left to the specified value.
hvac_seat_heater_right	Type: Integer Range: 0 to 3 Default: 0 Set the HVAC seat heater right to the specified value.
hvac_steering_wheel_heat	Type: Boolean Default: false Set the HVAC steering wheel heat to the specified value.
drive	
speed_limit_mode	Type: Boolean Default: false Set the speed limit mode to the specified value.
speed_limit_pin	Type: Integer Range: 0 to 9999 Default: 0 Set the speed limit pin to the specified value.
speed_limit_offset	Type: Integer Range: -32768 to 32767 Default: 0 Set the speed limit offset to the specified value.
software	
software_update_scheduled_start	Type: Integer Range: -32768 to 32767 Default: 0 Set the software update scheduled start to the specified value.
software_update_scheduled_end	Type: Integer Range: -32768 to 32767 Default: 0 Set the software update scheduled end to the specified value.
software_update_offset	Type: Integer Range: -32768 to 32767 Default: 0 Set the software update offset to the specified value.
security	
valet_mode	Type: Boolean Default: false Set the valet mode to the specified value.
valet_pin	Type: Integer Range: 0 to 9999 Default: 0 Set the valet pin to the specified value.
guest_mode	Type: Boolean Default: false Set the guest mode to the specified value.
sentry_mode	Type: Boolean Default: false Set the sentry mode to the specified value.
sentry_mode_notification	Type: Boolean Default: false Set the sentry mode notification to the specified value.
sentry_mode_blind_spot	Type: Boolean Default: false Set the sentry mode blind spot to the specified value.
pin_to_drive_enabled	Type: Boolean Default: false Set the pin to drive enabled to the specified value.
pin_to_drive_pin	Type: Integer Range: 0 to 9999 Default: 0 Set the pin to drive pin to the specified value.
driver_first	Type: Boolean Default: false Set the driver first to the specified value.
media	
media_volume	Type: Integer Range: 0 to 100 Default: 0 Set the media volume to the specified value.
media_playback_status	Type: Enumeration Allowed values: playing, stopped Default: stopped Set the media playback status to the specified value.
navigation	
nav_destination	Type: Blob Max length: 65535 Set the navigation destination to the specified value.
nav_waypoints	Type: Blob Max length: 65535 Set the navigation waypoints to the specified value.
nav_route	Type: Blob Max length: 65535 Set the navigation route to the specified value.
nav_supercharger_filter	Type: Boolean Default: false Set the navigation supercharger filter to the specified value.
nav_supercharger_filter_type	Type: Enumeration Allowed values: all, compatible, favorites, recent Default: all Set the navigation supercharger filter type to the specified value.
nav_supercharger_filter_fast	Type: Boolean Default: false Set the navigation supercharger filter fast to the specified value.
nav_supercharger_filter_amenities	Type: Boolean Default: false Set the navigation supercharger filter amenities to the specified value.
nav_supercharger_filter_exclude_full	Type: Boolean Default: false Set the navigation supercharger filter exclude full to the specified value.
nav_supercharger_filter_exclude_non_favorites	Type: Boolean Default: false Set the navigation supercharger filter exclude non favorites to the specified value.
nav_supercharger_filter_exclude_non_compatible	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible to the specified value.
nav_supercharger_filter_exclude_non_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non recent to the specified value.
nav_supercharger_filter_exclude_non_compatible_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible recent to the specified value.
nav_supercharger_filter_exclude_non_favorites_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non favorites recent to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent to the specified value.
nav_supercharger_filter_exclude_non_compatible_recent_favorites	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible recent favorites to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities exclude full to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full_exclude_non_favorites	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities exclude full exclude non favorites to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities exclude full exclude non favorites exclude non compatible to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities exclude full exclude non favorites exclude non compatible exclude non recent to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast to the specified value.
nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities to the specified value.
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nav_supercharger_filter_exclude_non_compatible_favorites_recent_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent_exclude_non_compatible_recent_exclude_non_favorites_recent_exclude_non_compatible_favorites_fast_amenities_exclude_full_exclude_non_favorites_exclude_non_compatible_exclude_non_recent	Type: Boolean Default: false Set the navigation supercharger filter exclude non compatible favorites recent fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent exclude non compatible favorites fast amenities exclude full exclude non favorites exclude non compatible exclude non recent exclude non compatible recent exclude non favorites recent to the specified value.
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pathwalker

Phanto *Active Linux Monitor* **M**ovements **O**bserved **N**etwork **T**ransmitted **O**ctopus **M**ultiprocess

Model building with Pathwalker

Author(s)

Jochen Bern, Phantom Raiser

Purpose

Build a mouse path walking

How pathwalker works:

Examples

Standard run of pathwalker:

Running pathwalker is easy. Finish the command line you can type:

```
./bin/pathwalker.py map.txt -resolution 3\resolution 2 -\scale 50
```

This will build a model based on the map my_map.txt at a resolution of 3 A using a threshold of 0.2 and building a scale of 50.

Possible Problems

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
usage: pathwalker [-h] [-v]
                  [-c CONFIG_FILE]
                  [-m MAP_FILE] [-l LOG]

optional arguments:
  -h, --help            show this help message and exit
  -v, --verbose         Verbosity level
  -c CONFIG_FILE, --config_file CONFIG_FILE
                        Path to a configuration file
                        (default: pathwalker.cfg)
  -m MAP_FILE, --map_file MAP_FILE
                        Path to a map file
                        (default: map.txt)
  -l LOG, --log LOG     Path to a log file
                        (default: pathwalker.log)

  --version             show program's version number and exit

  -p, --path            [ 0 | 1 ]
                        Path to walk
                        (default: 1)
  -w, --walk            [ 0 | 1 ]
                        Walk the path
                        (default: 0)
  -r, --resolution      [ 0 | 1 ]
                        Resolution of the map
                        (default: 1)
  -s, --scale           [ 0 | 1 ]
                        Scale the map
                        (default: 0)
  -t, --threshold       [ 0.0 | 1.0 ]
                        Threshold for the map
                        (default: 0.2)
  -d, --debug           [ 0 | 1 ]
                        Debug mode
                        (default: 0)
  -b, --build           [ 0 | 1 ]
                        Build the map
                        (default: 1)
  -g, --gnuplot         [ 0 | 1 ]
                        Use gnuplot
                        (default: 1)
  -f, --force           [ 0 | 1 ]
                        Force to overwrite existing files
                        (default: 0)
  -n, --name            [ 0 | 1 ]
                        Name of the map
                        (default: 1)
  -x, --x_step          [ 0.0 | 1.0 ]
                        Step size in x direction
                        (default: 0.1)
  -y, --y_step          [ 0.0 | 1.0 ]
                        Step size in y direction
                        (default: 0.1)
  -a, --angle           [ 0.0 | 360.0 ]
                        Angle of the path
                        (default: 0.0)
  -o, --output          [ 0 | 1 ]
                        Output
                        (default: 1)
  -i, --input           [ 0 | 1 ]
                        Input
                        (default: 0)
  -e, --error           [ 0 | 1 ]
                        Error
                        (default: 1)
  -u, --usage           [ 0 | 1 ]
                        Usage
                        (default: 0)
  -h, --help            [ 0 | 1 ]
                        Help
                        (default: 0)
  -v, --version         [ 0 | 1 ]
                        Version
                        (default: 0)
  -c, --check           [ 0 | 1 ]
                        Check
                        (default: 0)
  -m, --map             [ 0 | 1 ]
                        Map
                        (default: 0)
  -l, --log             [ 0 | 1 ]
                        Log
                        (default: 0)
  -p, --path            [ 0 | 1 ]
                        Path
                        (default: 0)
  -w, --walk            [ 0 | 1 ]
                        Walk
                        (default: 0)
  -r, --resolution      [ 0 | 1 ]
                        Resolution
                        (default: 0)
  -s, --scale           [ 0 | 1 ]
                        Scale
                        (default: 0)
  -t, --threshold       [ 0.0 | 1.0 ]
                        Threshold
                        (default: 0.0)
  -d, --debug           [ 0 | 1 ]
                        Debug
                        (default: 0)
  -b, --build           [ 0 | 1 ]
                        Build
                        (default: 0)
  -g, --gnuplot         [ 0 | 1 ]
                        Gnuplot
                        (default: 0)
  -f, --force           [ 0 | 1 ]
                        Force
                        (default: 0)
  -n, --name            [ 0 | 1 ]
                        Name
                        (default: 0)
  -x, --x_step          [ 0.0 | 1.0 ]
                        X step
                        (default: 0.0)
  -y, --y_step          [ 0.0 | 1.0 ]
                        Y step
                        (default: 0.0)
  -a, --angle           [ 0.0 | 360.0 ]
                        Angle
                        (default: 0.0)
  -o, --output          [ 0 | 1 ]
                        Output
                        (default: 0)
  -i, --input           [ 0 | 1 ]
                        Input
                        (default: 0)
  -e, --error           [ 0 | 1 ]
                        Error
                        (default: 0
```

pdbtools

Phenix *Python based Hierarchical Environment for Integrated Xtallography*

phenix.pdbtools: PDB model manipulations and statistics

Contents:

- Manipulations on a model in a PDB file including
- Command line
- Graphical interface
- Command line
- List of all available keywords

Manipulations on a model in a PDB file including

The operations listed can be applied to the whole model or selected parts (e.g. chain(s),selection=chain A and resnum 1:10 and resname ala).

- remove hydrogen atoms
- replace chemical elements (element xxxfrom xxxto)
- remove alternate conformations
- set occupancies to one
- set occupancies to zero
- set occupancies to a value
- setting of B-factor (isotropic or anisotropic)
- setting of B-factor to a constant value
- setting of B-factor to a random value (between 1 and 100)
- setting of B-factor to a random value (between 1 and 100) proportional to the value of occupancy
- setting of B-factor to the value of occupancy
- renumbering of residues
- renumbering of chains
- change chain identifiers
- change residue identifiers
- change atom identifiers

Video Tutorial

The youtube page is available on the Phenix YouTube channel and covers the following topics:

- basic overview
- Phenix GUI interface via the GUI
- Phenix command line interface along with more interactive data
- example 1: selection of a sequence in a model in phenix

Graphical interface

As usual, one is able to use appropriate geometry restraints for refinement and refinement strategies. (This parameters are not shown in the screenshot but can be selected this way. Take into account that some options are not always recommended.) Partial symmetry is not essential but also recommendable, and will be propagated to the output model.

Many different options are possible, only some of which are shown in the main window. The atom selection controls can be used to specify which part of the model will be affected by various changes, or to eliminate parts of the model. The standard selection syntax is Phenix-specific, but examples are shown in the selection editor dialog.

Hint: In case anyone PDBTools was also responsible for generating chemical/bond and additions of hydrogen atoms, the following options are available: Generate hydrogen atoms (polar/all), chemical/bond and Phenix/Reduce add hydrogen.

Command line use

Phenix.pdbtools

1) Type phenix.pdbtools from the command line for instructions:

```
phenix.pdbtools
```

2) To see all default parameters:

```
phenix.pdbtools --show-defaults
```

3) Response a PDB model consist of three chains A, B and C and some water molecules. Remove all atoms in chain B and write out:

```
phenix.pdbtools model.pdb remove="chain C or water"
```

or one can achieve exactly the same result with equivalent command:

```
phenix.pdbtools model.pdb keep="chain A or chain B"
```

or

```
phenix.pdbtools model.pdb keep="chain A or water"
```

or finally:

```
phenix.pdbtools model.pdb remove="chain C or chain B"
```

4) Change the occupancies of all atoms in chain A to zero:

The chain A in the example below will remain where all atoms have occupancies equal to one.

```
phenix.pdbtools model.pdb occupancy.set=0 selection="chain A"
```

5) Remove all water and set all B-factors to 20:

```
phenix.pdbtools model.pdb remove=water b_iso.set=20
```

6) Change the occupancies of all atoms in chain A and water water molecules. Remove all but water. Remove all B-factors and set B-factor to value of occupancy:

```
phenix.pdbtools model.pdb keep=water occ.set=0.5 selection="chain A"
```

List of all available keywords

```
model
  remove = None                       Selection for the atoms to be removed
  keep = None                         Select atoms to keep
  selection = chain pdb_test          Selection for the scope of mod.
  selection = None                    Selection for atoms to be modified
  output
    prefix = None                     Prefix
    change_of_hand = False            Flip symmetry where applicable
    overwrite = True                  Overwrite existing files
    scale_to_unit_cell = False        Scale output to unit cell
    crystal_symmetry = None           Write symmetry with unit cells
    cif = False                       Output in mmCIF format
    cif_ext = None                    Extension for mmCIF files
    pdb = True                        Output in PDB format
    pdb_ext = None                    Extension for PDB files
    output_file_name = None           Full output PDB file name
    remove_ss_records = False         Do not write any SS records (HELIX or
                                      SHEET) to the output file
    remove_cryst_and_scale_records =  Do not write any CRYST1, SCALE1, SCALE2
    False                             or SCALE3 records to the output file
    write_hydrogens = False           Write hydrogen atoms
    write_ter_records = False         Write TER records
    write_hetatm_records = False      Write HETATM records
    write_model_records = False       Write MODEL/ENDMDL records
    write_single_model = False        Write only the first model to the output
    write_pdb_to_stdout = False       Write PDB output to stdout
    write_cif_to_stdout = False       Write CIF output to stdout
    write_hkl_to_stdout = False       Write HKL output to stdout
    write_mtz_to_stdout = False       Write MTZ output to stdout
    write_ncs_to_stdout = False       Write NCS output to stdout
    write_geo_to_stdout = False       Write GEO output to stdout
    write_cif_to_stdout = False       Write CIF output to stdout
    write_hkl_to_stdout = False       Write HKL output to stdout
    write_mtz_to_stdout = False       Write MTZ output to stdout
    write_ncs_to_stdout = False       Write NCS output to stdout
    write_geo_to_stdout = False       Write GEO output to stdout
    write_cif_to_stdout = False       Write CIF output to stdout
    write_hkl_to_stdout = False       Write HKL output to stdout
    write_mtz_to_stdout = False       Write MTZ output to stdout
    write_ncs_to_stdout = False       Write NCS output to stdout
    write_geo_to_stdout = False       Write GEO output to stdout
  sites
    shift = None                      Shift to be applied to all atoms
    rms_randomization = None          Add random noise to atom positions with
                                      specified RMS deviation
    random_seed = None                Seed for generating random shifts
    apply_to_hydrogens_too = False    Apply shift to hydrogen atoms as well
  occupancy
    remove = None                     Selection for atoms to be removed
    keep = None                       Selection for atoms to be kept
    selection = chain pdb_test        Selection for the scope of occupancy
    selection = None                  Selection for atoms to be modified
    set = None                        Set all or selected occupancies to given value
    randomize = False                 Randomize occupancies
    random_seed = None                Seed for generating random shifts
    rms_deviation = None              Add random noise to atom occupancies with
                                      specified RMS deviation
    rms_deviation_to_average = None   Add random noise to atom occupancies with
                                      specified RMS deviation from average
    rms_deviation_to_value = None     Add random noise to atom occupancies with
                                      specified RMS deviation from specified value
    invert = False                    Invert occupancies
    multiply_by = None                Multiply occupancies by a factor
    add = None                        Add to occupancies
    occupancy_threshold = None        Set occupancies below this threshold to
                                      zero
    remove_if_occupancy_zero = False  Remove atoms with zero occupancy
  b_iso
    remove = None                     Selection for atoms to be removed
    keep = None                       Selection for atoms to be kept
    selection = chain pdb_test        Selection for the scope of B-iso
    selection = None                  Selection for atoms to be modified
    set = None                        Set all or selected B-iso to given value
    randomize = False                 Randomize B-iso
    random_seed = None                Seed for generating random shifts
    rms_deviation = None              Add random noise to B-iso with specified
                                      RMS deviation
    rms_deviation_to_average = None   Add random noise to B-iso with specified
                                      RMS deviation from average
    rms_deviation_to_value = None     Add random noise to B-iso with specified
                                      RMS deviation from specified value
    invert = False                    Invert B-iso
    multiply_by = None                Multiply B-iso by a factor
    add = None                        Add to B-iso
    b_iso_threshold = None            Set B-iso below this threshold to zero
    remove_if_b_iso_zero = False      Remove atoms with zero B-iso
  b_aniso
    remove = None                     Selection for atoms to be removed
    keep = None                       Selection for atoms to be kept
    selection = chain pdb_test        Selection for the scope of B-aniso
    selection = None                  Selection for atoms to be modified
    set = None                        Set all or selected B-aniso to given value
    randomize = False                 Randomize B-aniso
    random_seed = None                Seed for generating random shifts
    rms_deviation = None              Add random noise to B-aniso with specified
                                      RMS deviation
    rms_deviation_to_average = None   Add random noise to B-aniso with specified
                                      RMS deviation from average
    rms_deviation_to_value = None     Add random noise to B-aniso with specified
                                      RMS deviation from specified value
    invert = False                    Invert B-aniso
    multiply_by = None                Multiply B-aniso by a factor
    add = None                        Add to B-aniso
    b_aniso_threshold = None          Set B-aniso below this threshold to zero
    remove_if_b_aniso_zero = False    Remove atoms with zero B-aniso
  element
    atom_selection = None             Selection for atoms to be changed
    element = None                    Element to be assigned
  rotate_about_axis
    axis = None                       Axis to be used for rotation
    angle = None                      Angle of rotation
    atom_selection = None             Selection for atoms to be rotated
  translate
    shift = None                      Translation vector
    atom_selection = None             Selection for atoms to be translated
  rotate_about_axis
    axis = None                       Axis to be used for rotation
    angle = None                      Angle of rotation
    atom_selection = None             Selection for atoms to be rotated
  set_charge
    atom_selection = None             Selection for atoms
    charge = None                     Charge
```

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

Rapid phase improvement and model-building using phase_and_build

Contents

- Authors
- Usage
- Output
- Phase_and_build.exe
- Parameters files phase_and_build
- Parameters files phase_and_build
- Examples
- Standard run of phase_and_build.
- Specific limitations and problems:
- Literature
- Additional information

Author(s)

Thomas Ashton, Tom Terwilliger

Purpose

phase_and_build is a new and rapid method for improving the quality of your map and building a model. The approach is based on an iterative procedure of density modification and model building. The density modification is carried out using the phenix.density_modification program. The model building is carried out using phenix.ellmen a new in phenix automatic tool which was used on building the best possible model of each image. The ellmen tool is described in detail in the paper Ashton et al. (2020). The phase_and_build tool is a wrapper that runs a number of other phenix programs. The phenix.phase_and_build program takes a map and a sequence file and uses a number of other phenix programs to produce a model and improved map.

Usage

How phase_and_build works:

phase_and_build first identifies a feel set of reflections if they are not supplied. It uses without the feel set reflections to calculate a phase probability distribution. It set of data for density modification is created which contains phenix.ellmen formatted files (if supplied).

- Next phase_and_build estimates the variant fraction (if not supplied) from the sequence file and cell dimensions using phenix.molecular_weight. This is used in the density modification.
- A phase map is obtained by density modification of the input data using a map coefficients file in phenix.ellmen.
- The phase map is used to create a model using phenix.ellmen. This is run using a default time of 1 hour unless the time is supplied. NCS and that the sequence file are used in building. A partial model is created and the model is used to calculate a map using phenix.map_to_model.
- Next the phase probability distribution is calculated using the model and the phase map.
- Next the phase probability distribution is used to create a new map using phenix.fmodel. This map is used in the next cycle of density modification. The phase probability distribution is used in the density modification to create a new map.
- The process is repeated for a number of cycles (default is three recent map). One or more models are from each cycle of density modification and model building are combined using phenix.combine_models. The combining method is default and separate models are combined after each cycle of density modification and model building. The final model is refined using phenix.fmodel. Output and the final model is refined and phenix.refine.

Output files from phase_and_build

phase_and_build.sh is the top level run script. Invoke **phase_and_build.map_coeffs.sh** to MTZ file phase_and_build_map_coeffs.mtz and **phase_and_build.sh** to run phase_and_build.

Parameters files in phase_and_build

phase_and_build.sh and phase_and_build.map_coeffs.sh phase_and_build uses all parameters file that can be used on your phenix phase_and_build and is a wrapper of phenix.ellmen, phenix.molecular_weight, phenix.fmodel, phenix.density_modification, phenix.map_to_model, phenix.combine_models and phenix.refine. phenix.phase_and_build.sh the temporary directory used in building. You can use these with:

```
phenix.phase_and_build.sh --ncs=ncs.ncs_spec --seq_file=seq.seq --resolution=2.0 --cycles=3 --time_limit=1 --nproc=4 --ncs_copies=6 --variant_fraction=0.5 --phase_and_build_dir=phase_and_build_dir --ellmen.ellmen.n_cycle_build_max=3 --ellmen.ellmen.n_cycle_rebuild_max=0 --ellmen.ellmen.n_cycle_refine_max=0 --ellmen.ellmen.n_cycle_ncs_copies_refine_max=0 --ellmen.ellmen.n_cycle_ncs_copies_refine_min=0 --ellmen.ellmen.n_cycle_rebuild_max=0 --ellmen.ellmen.n_cycle_refine_max=0 --ellmen.ellmen.n_cycle_ncs_copies_refine_max=0 --ellmen.ellmen.n_cycle_ncs_copies_refine_min=0 --ellmen.ellmen.n_cycle_build_max=1
```

phenix

Automated Molecular Replacement with Phaser

Contents

- Automated Molecular Replacement
- Phaser Release Notes 2.1
- Phaser Release of Data should be used
- Phaser Tutorial
- Phaser FAQ
- Phaser Log to Cif/Mmcif Utility
- How to Define Data
- Phaser Log Parser
- Phaser Log Parser Cross Rot Coordinates
- Phaser Log Parser Cross Rot Data
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  - Connection to Sculptor Tutorial
  - Connection to Sculptor Tutorial Phenix.xtriage
  - Connection to Sculptor Phenix.refine
  - Connection to Sculptor Phenix
  - Connection to Sculptor Coot
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  - PDB Clustering
  - Cluster Analysis Tutorial
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  - Phaser Rot selection and packing
  - Phaser Tf selection
  - Phaser Ll selection
  - Phaser Tfz selection
  - Phaser Tfz Rfz
- Phaser Rotation Function Scriptable
- Phaser Tf Rfz
- Phaser Ll Rfz
-

Fig.(1)

How to Control Output

The output of Phaser can be controlled with optional keywords.

Phaser has a number of keywords which are prefixed by a keyword ("PHASER"), but should always be given, so that you can have separate and meaningful output filenames.

The TOPAS keyword controls the number of potential MR solutions for which FSR and LLG the aggregates are calculated. The default is 1.

For the MR SHELL MR DRF and MR LLG modes, where PHASER DRF is given as an optional keyword, Phaser calculates the Rotation Function using the Fourier Method. The following keywords control scattering factor details as follows:

Keyword	**Description**
NOFOURIERFACTORS	Amplitude and phase for $\Sigma\Sigma\Sigma$ $f_{jm}F_{hkl}$ and $W_{jm}F_{hkl}$ ~ time
NOFOURIERFACTORS	Amplitude and phase for $\Sigma\Sigma\Sigma$ $f_{jm}F_{hkl}$ and $W_{jm}F_{hkl}$ ~ time
LLG	for analysis in the TFZ* LLGain, to optimize the reliability of LLG
NOFRACTIONALTOL	Fractional cartesian coefficient rounding for phase probability distribution

Translational Non-crystallographic Symmetry

"Warning! Solution by MR in the presence of translational non-crystallographic symmetry is not fully supported.

Phaser calculates correlation blocks for the expected intensities in the presence of translational non-crystallographic symmetry. **Phaser does not yet have a full set of tests for this case. Because the use of Phaser in the presence of NCS requires the nature of the NCS to be understood by the user, Phaser does not yet have a full automated procedure for dealing with NCS. Phaser does not yet have a full set of tests for the case of translational NCS.**

Phaser does not yet work with the case of translational pseudo-NCS, but **the NCS is not completely characterized by Phaser.** The default behaviour may or may not be correct for the particular case of pseudo-NCS.

Characterization of the NCS involves understanding the number of copies of the molecule in the asymmetric unit, and the translations between the molecules. Knowledge of the NCS allows the user to specify the expected peak heights for the Patterson. Phaser calculates the expected peak heights for the Patterson, and the user can see these in the Patterson Function output. Phaser will also find the peaks in a list of peaks passed matching the criteria.

Default INCS detection and correction

Documentation for Phaser-2.7.16 and above

No INCS

No INCS correction is applied by default if there is

1) no peak in the native Patterson
2) no intermolecular vectors between over 20% of the origin and three peaks are not at the result of intermolecular vectors

Pairs of molecules

By default, if Phaser detects a peak in the native Patterson then Phaser will search for molecules in pairs related by the NCS, and will use the NCS in the calculation.

This will be the correct behaviour if and only if there are an even number of copies of the molecule in the asymmetric unit, between the pairs related by a single NCS vector. There will only be one significant peak in the Patterson, and the NCS will be a 2-fold rotation-translation.

Phaser checks the relative orientation of the molecules in the two groups (copies) of six to 20 degrees and will not use the NCS if the molecules are too similar. Phaser will also not use the NCS if the NCS vector is too close to the crystallographic. Solution should be straightforward with the usual cause for MR that there is a sufficiently large model.

Where there is a single peak in the native Patterson, it is often located at a position that was along a cell edge in the Patterson of the model, and the peak is at a position that is not at the origin. This is a common case for translational NCS. Phaser checks for this case, and will not use the NCS, and the NCS vector can be in a general position.

Non-default INCS correction

Higher order INCS

Frequently, NCS does not associate 2 copies of molecules in the asymmetric unit, but rather there are 3 or more (or fraction of molecules associated in a whole or unrounded sub-multiple of 1, 2 , 3 , or 4) copies in the asymmetric unit. Phaser will find the NCS vector, and will find the peaks in the Patterson, but will not find the relative orientations of the molecules, and will not associate 3 or more copies of the molecule.

Phaser will also not associate 3 or more copies of the molecule. The pairwise translational relationships are analysed to find the 3-fold relationship. The sense will not generally have all peaks the same height. Lower peaks will be at the positions of the higher peaks multiplied by the rotation-translation. Phaser will find the relative orientations of the molecules, but will not find the relative orientations of the molecules, and will not associate 3 or more copies of the molecule.

Phaser does use TNCS INFO, and the vector for the INCS, and searches for anomalies in multiples of INFO.

Phaser will find the relative orientations of the molecules related by INCS, Phaser does not refine the orientations between the molecules related by the NCS.

However, as for two-fold INCS, Phaser is not optimized to deep sorts of pseudo-cells and the base INCS vector will be in a general position, and will not be in a special position.

The automatic detection may not give the true INCS relationship. For example, the true commensurate relationship may be a 3-fold, but the peaks in the Patterson may be at the positions of the 2-fold relationship, or at a commensurate relationship may be the base with the defined Patterson peak height could be a fraction of the peak height in the Patterson for peaks.

Complex INCS

If there are many molecules in the asymmetric unit but they are not all related by NCS, or there are two groups of molecules related by different NCS, Phaser does not find the relative orientations of the molecules, and will not find the relative orientations of the molecules. **Phaser does not yet provide the user with a procedure to specify the NCS relationships. Phaser does not yet provide the user with a procedure to specify the NCS relationships.**

Phaser does not yet have a full set of tests for the case of complex NCS. Phaser does not yet have a full set of tests for the case of complex NCS.

In the case of two NCS relationships between the molecules, the peaks in the Patterson will be complex and difficult to interpret. Phaser does not yet have a procedure to deal with this case.

Consider the highest native Patterson peak that will determine the vector of the NCS associated with it. Use the Patterson Function output to find the peaks associated with the NCS. Use the Patterson Function output to find the peaks associated with the NCS. Use the Patterson Function output to find the peaks associated with the NCS. Find the relative orientations of the molecules, using the peaks. Set up the NCS files with the relative orientations.

phase_rp

SAD and MR-SAD phasing with the Phaser GUI

Contents

- Introduction
- Input files and mandatory parameters
- Output
- Frequently Asked Questions
- References

Introduction

Since the last Phaser DUG was a common topic, much of the experimental phasing interface is similar to the Phaser-EP GUI. Please read the Phaser-EP GUI documentation for more detailed information on the GUI.

Phaser is used internally in the autosol script, which automates a complete experimental phasing pipeline, including SAD phasing, density modification, model building and refinement. Although the GUI is not capable of running MR-SAD experiments (LLG Full Gradient, see recommended trying Autofrost first), and PDBs back to Phaser cannot be used, it is still a useful tool for visualizing and manipulating phasing results.

This document only covers configuration of the Phaser GUI. For a detailed explanation of the various terms and special commands mentioned, see as well as interpretation of results, consult the documentation for Phaser or Phaser-EP, and the Phaser DUG.

Input files and mandatory parameters

Phaser requires a reflections file (one format containing anomalous data, and the normal SAD model is the recommended input format), a sequence file, and a PDB file containing the substructure (if one is known, if not see below). If you are using Phenix Bash Scripts, one may choose whether to use the gaussian ensemble ("Fast(G)") or the Full Gradient ("Full LLG") target function.

To run an MR-SAD experiment, change the mode to "MR-SAD phasing", and enter a partial model (PDB file) and the sequence of the target molecule. Phaser will then perform a rotation function, and place the partial model relative to the cell and scattering. For more complicated cases, or for a phasing library of partial models, one may use the Phaser Expert Mode to run a translation function, or a rotation function followed by a translation function (generally recommended for the same level and reason as the rotation mode). Phaser will then output a PDB file containing the solution, which can be used as input for refinement and model building. Change "Fast(G)" to "Full LLG" for "Full Gradient" target function.

The Fast MR-SAD scheme is derived in the Phaser-TNG paper. There seems little difference between the Fast(G) and Full LLG target functions, but the Fast(G) target function is faster.

Output

Depending on the choice of tools, Phaser will output one or two sets of files containing the heavy atom sites (PDB/mtz). Phaser-EP will output a set of files containing the refined heavy atom sites, and a set containing the anomalous difference peaks (for phasing with isomorphous/anomalous difference). This may be useful very large structures, where one may want to use the anomalous difference peaks in reporter sites.

Frequently Asked Questions

- **How do I tell Phaser to look for cross anomalous scatterers?** Click on the "Computation Mode" button, and change the mode to "Anomalous Difference Fourier". Change the "Anomalous scattering atoms" tab to the element, and to anyone, e.g. selenium. Expected Phaser-EP output will be a set of files containing the refined heavy atom sites, and a set containing the "Anomalous peaks" (for either isomorphous or using the "Difference Anomalous Peaks" button. The "Anomalous peaks" can be used as input for substructure search programs, such as Phenix Hybrid Substructure Search or Crunch2 (Crunch2 can also be used for substructure modelling, some Phenix tools can also read Crunch2 output).
- **How do I phase a structure with lanthanide bromide clusters in Phenix?** This is possible, but requires some manual work. Phaser-EP can find the lanthanide sites, and output a PDB file with the lanthanide sites. The cross anomalous peaks can be used as input for substructure search programs. The cross anomalous peaks can also be used as input for refinement, and the lanthanide sites can be used as input for refinement. The output PDB can be refined in Phenix or Coot to produce bromine sites.

References

- McCoy AJ, Grosse-Kunstleve RW, Adams PD, Winn MD, Storoni LC, Read RJ. Phaser crystallographic software. J Appl Cryst. (2007) 40:658-674.
- Terwilliger TC, Adams PD, Read RJ, McCoy AJ, Moriarty NW, Grosse-Kunstleve RW, Afonine PV, Oeffner RD, Oeffner RD. Decision-making in structure solution using Bayesian estimates of map quality: the PHENIX AutoSol wizard. Acta Cryst D. (2009) 65:582-601.

phaser_mr

Molecular replacement with the Phaser GUI

Contents

- Overview
- Video Tutorial
- Input files and mandatory parameters
- Additional parameters
- Re-using previous results
- Frequently Asked Questions
- Reference

Overview

Phaser presents a user-friendly and automated framework in Phaser but especially difficult cases may require finer control over parameters. The Phaser MR GUI exposes all options available in the standalone command line interface and allows the user to control the parameters of the search. The GUI also allows the user to run a series of searches in a variety of ways, including alternate space group and possible ensembles, or to edit output of the search (rotation or translation) and continue with further searches.

There is also a simplified GUI for structures with only one component in the cluster, allowing the relevant files to be selected and the search to be run with default options. This is described in the Phaser Simple GUI tutorial.

The Phaser MR GUI provides a graphical configuration of the Phaser GUI for a standard application of the various tools and search procedures referenced here as well as interpretation of results. Install the Coordinate or Ensemble Manipulation GUI to view results of Phaser MR searches. Phaser MR can also be used to prepare input for Molecular Replacement with Phaser MR. Many more options are available on the command line or the Phaser options and Phaser MR GUI. Phaser MR is a GUI for the Phaser Molecular Replacement and Phaser Ensemble Generation programs.

Video Tutorial

The tutorial video is available on the Phenix YouTube channel and covers the following topics:

- Phaser overview
- Phaser MR using the Phaser GUI

Input files and mandatory parameters

The input section is similar to that of Phaser, with separate sections for reflection data, search ensembles, and output files. Mandatory parameters are the reflection data, at least one ensemble, and the output prefix. Optional fields are then provided and automatically filled, or alternate options can be chosen from the drop-down menus. The Phaser MR GUI allows the user to specify the number of solutions to be found, the number of components in the cluster, and other parameters displayed.

All models require a description of the search ensemble, either an PDB file (single, or superimposed) or an ensemble in the Phaser format. Ensembles can be created using the Ensemble Manipulation GUI, and multiple ensembles can be specified which will be tried in turn (one ensemble at a time). Ensembles for a chain, and chain Phaser to try each in turn (all labeled).

Phaser MR allows the user to specify the number of components in the cluster (likely to positively information about the deposition and ideal of chains, heavy, or ligand and number of residues. Alternatively, the user can specify the number of residues in the cluster, and Phaser will try to find the number of residues in the cluster. Phaser does find contributed to scattering, but this is rarely necessary. Note that the SAD contents data does not contribute to the scattering, and Phaser will not find the number of SAD sites. Phaser will find the number of residues and use the number of residues in the cluster. Phaser will find the number of residues and use the number of residues in the cluster. Phaser will find the number of residues and use the number of residues in the cluster. Phaser will find the number of residues and use the number of residues in the cluster.

Finally, the "Search ensemble" tab defines the steps in the MR search, selected from each search ensemble. The number of steps can be specified, and the search ensemble to be used in each step. Alternatively, the number of steps is specified and the search ensemble chosen randomly, or ensembles can be specified to be tried in turn. Ensembles in combination ensembles from all the parts of the search ensemble. Specifying more than one ensemble in a search step will cause Phaser to try all combinations of the ensembles in the search step. Phaser will search for all combinations, or alternatively, Phaser.

Search
Search ensemble
Search ensemble
Search ensemble

Phenix *Python-based Hierarchical Environment for Integrated Bibliography*

phenix.maps: Command-line tool to compute various maps and save them to novel or global formats

How to run the command-line tool:

1. Create a parameter file (default name phenix.maps.parameters) using the command-line option --write-parameter-file. This will create a parameter file called maps.phenix.maps.parameters. Alternatively, you may specify input files (and additional parameters) directly on the command-line.
2. Edit the parameter file as needed.
3. Run the command-line tool: phenix.maps maps.parameters

Alternately, you may specify input files (and additional parameters) directly on the command-line:

phenix.maps model.pdb data.mtz

and it will automatically upscale the defined maps as described above.

Important Note:

- phenix.maps is available in PHENIX 2010
- phenix.maps uses a new "map coefficients" format defines the map that will be output as Fourier map coefficients. The scope of parameters "map" defines the maps that will be output as CCP4 or Fourier coefficients.
- To make maps from the command-line, the parameter file must contain at least one "map" section. Without any "map" sections, no maps will be output. You can use a file of defaults to define the "map" sections if you do not want to specify them on the command-line.
- A map is defined by specifying a map type using 'map_type' keyword available within each "map" section. Available map types are: 2mfo-dfc, mfo-dfc, anomalous, omit, mfo, mfo-mfo, and fo-fc. Alternatively, "Phase" for example, or "fo, sigma-sigma" for a phase-weighted map. Map coefficients for the specified map will be output in the Fourier coefficient file. Separated.
- Phenix.maps creates as many files with CCP4 or A.ion formatted maps as is requested, and it creates one Fourier coefficient file containing all requested map coefficients.
- The name of a CCP4 formatted map can be composed of the prefix and suffix of around selected atoms.
- Twinning ID detection will be automatted for automatically. This can be disabled by using "twinning_detection=false" on the command-line.
- All values used in map calculation, for example, Mtrix, Fmodel, Fom, Fmean, A, B, etc, can be output in the Fourier coefficient file if desired.
- For three-wire data no experiment, bulk solvent correction and anisotropic scaling can be turned off using the "no_scaling" command-line option.
- Phenix.maps can be used to calculate maps using a pdb file and a reflection file with no model. Specifically, the "model" keyword can be omitted and the "reflections" keyword used.
- Phenix.maps can be used to calculate maps using a pdb file and a reflection file with no model.
- For ccp4 map calculation, if you specify the wavelength and working heavy atoms (if or heavier) with the keywords "wavelength" and "heavy_atoms" using the Phenix.refine syntax, phenix.maps will use the Bijvoet contribution to the anomalous map.

phenix.maps parameters:

```
phenix.maps {
  maps {
    map_coefficients {
      file_name = None
      directory = None
      output_format = Mtrz
      exclude_free_r_flags
      fill_missing_flags
      scale_to_fobs = True
      remove_sigma_cutoff
      remove_sigma_cutoff = True
      fill_missing_flags
      fill_missing_flags = True
      scale_to_fobs
      scale_to_fobs = True
      output_ccp4_map = False
      ccp4_map {
        map_type = 2mfo-dfc | mfo-dfc
        map_coefficients_file_name = None
        grid_resolution = None
        scale = None
        sigma_cutoff = None
        fill_value = None
        fill_value_ccp4 = None
        fill_value_xplor = None
        output_directory = None
      }
    }
    ccp4_map {
      directory = None
      prefix = None
      suffix = None
      map_type = 2mfo-dfc
      grid_resolution = None
      scale = None
      sigma_cutoff = None
      fill_value = None
      fill_value_ccp4 = None
      fill_value_xplor = None
      output_directory = None
    }
    xplor {
      directory = None
      prefix = None
      suffix = None
      map_type = 2mfo-dfc
      grid_resolution = None
      scale = None
      sigma_cutoff = None
      fill_value = None
      fill_value_ccp4 = None
      fill_value_xplor = None
      output_directory = None
    }
    anomalous {
      directory = None
      prefix = None
      suffix = None
      map_type = anom
      grid_resolution = None
      scale = None
      sigma_cutoff = None
      fill_value = None
      fill_value_ccp4 = None
      fill_value_xplor = None
      output_directory = None
    }
    omit {
      directory = None
      prefix = None
      suffix = None
      map_type = omit
      grid_resolution = None
      scale = None
      sigma_cutoff = None
      fill_value = None
      fill_value_ccp4 = None
      fill_value_xplor = None
      output_directory = None
    }
    mfo {
      directory = None
      prefix = None
      suffix = None
      map_type = mfo
      grid_resolution = None
      scale = None
      sigma_cutoff = None
      fill_value = None
      fill_value_ccp4 = None
      fill_value_xplor = None
      output_directory = None
    }
    mfo-mfo {
      directory = None
      prefix = None
      suffix = None
      map_type = mfo-mfo
      grid_resolution = None
      scale = None
      sigma_cutoff = None
      fill_value = None
      fill_value_ccp4 = None
      fill_value_xplor = None
      output_directory = None
    }
    fo {
      directory = None
      prefix = None
      suffix = None
      map_type = fo
      grid_resolution = None
      scale = None
      sigma_cutoff = None
      fill_value = None
      fill_value_ccp4 = None
      fill_value_xplor = None
      output_directory = None
    }
    fo-fc {
      directory = None
      prefix = None
      suffix = None
      map_type = fo-fc
      grid_resolution = None
      scale = None
      sigma_cutoff = None
      fill_value = None
      fill_value_ccp4 = None
      fill_value_xplor = None
      output_directory = None
    }
    phase {
      directory = None
      prefix = None
      suffix = None
      map_type = phase
      grid_resolution = None
      scale = None
      sigma_cutoff = None
      fill_value = None
      fill_value_ccp4 = None
      fill_value_xplor = None
      output_directory = None
    }
    fo, sigma-sigma {
      directory = None
      prefix = None
      suffix = None
      map_type = fo, sigma-sigma
      grid_resolution = None
      scale = None
      sigma_cutoff = None
      fill_value = None
      fill_value_ccp4 = None
      fill_value_xplor = None
      output_directory = None
    }
  }
}
```

Planning a SAD experiment with plan_sad_experiment

Author(s)

- plan_sad_experiment: Yun Tenebrae

Purpose

plan_sad_experiment is a tool for estimating the anomalous signal that you might get from your SAD experiment before actually performing the experiment. It also helps you to decide how many data sets to collect and how many anomalous sites should be refined anomalous sites to use in SAD phasing with SHELXC/D/E and AutoSHARP based on the estimated anomalous signal strength.

Usage

How plan_sad_experiment works:

- The square root of plan_sad_experiment calculates a sequence file, the anomalous scattering atom plus other to use for SHELXC/D/E and AutoSHARP based on the estimated anomalous signal.
- plan_sad_experiment also generates the minimum Crystal size of your datasets to provide enough anomalous signal for successful phasing.
- plan_sad_experiment will ask for various values of Crystal size (average & sd) of special mosaicities, the wavelength, the number of anomalous scatterers in the asymmetric unit, the number of data sets, the number of anomalous sites to refine, the resolution limit, the number of residues in the asymmetric unit, the number of anomalous scatterers and the number of data sets to use for SHELXC/D/E and AutoSHARP.
- plan_sad_experiment will then calculate the anomalous signal strength, the number of anomalous sites to refine, and the resolution limit for the square root of the Correlation of Effect. Then plan_sad_experiment will choose a value of Crystal Size that will give the anomalous signal strength and the number of anomalous sites to refine.
- Please note that plan_sad_experiment and anomalous signal estimate are only approximate. Actual values of anomalous signal and number of anomalous sites to refine may differ from the estimated values. Also, the number of data sets to use for SHELXC/D/E and AutoSHARP may differ from the number of data sets you actually collected. plan_sad_experiment will only provide a guideline for the anomalous signal and number of anomalous sites to refine.
- plan_sad_experiment will also provide the number of data sets to use for SHELXC/D/E and AutoSHARP based on the estimated anomalous signal. plan_sad_experiment will also provide a guideline for the number of data sets to use for SHELXC/D/E and AutoSHARP.
- plan_sad_experiment will also provide the minimum Crystal size to provide enough anomalous signal for successful phasing.

Output from plan_sad_experiment

plan_sad_experiment provides a summary of the scattering expected from your crystal and a summary of the anomalous signal expected from your crystal. It also provides the number of data sets to use for SHELXC/D/E and AutoSHARP based on the estimated anomalous signal. You can add the maximum Crystal to Tank Ratio to see examples setting max_crystal_size=20.

```
~~~
```

PHENIX

Python-based Hierarchical ENvironment for Integrated Xtallography

Generating a polder maps

Contents

- Overview
- Running the program
- Video Tutorial
- How to interpret the output .log file
- Examples
- Generating a polder map (command line)
- Other options
- Limitations
- List of available keywords

Overview

A polder map is an omit map which excludes the bulk solvent around the omitted region. This way, weak density features in the omitted region are not masked by the surrounding bulk solvent. Features that may be revealed by a polder map include:

- ligands
- water molecules occupying the ordered sites and with unclear alternate conformations (such as ions, acetylene, etc.)
- ordered bulk solvent features

It is not recommended to use large portions of the model or even the entirely bulk solvent volume might be excluded, which may lead to artifacts in the bulk solvent region or in the vicinity of the bulk solvent. For polder maps, it should be kept in mind that above certain dose (high crystallinity), no bulk solvent strategies may be sufficient to remove the bulk solvent signal.

A presentation file with examples can be found here.

Running the program

phenix.polder can be executed on the GUI, or the command line:

```
phenix.polder model.pdb data.mtz selection="chain A"
```

The output files will be written to the current directory. The output files for the formats are suffixed .pdb and .cif for models, .map, .ccp4 for maps. The default for the selection is the same as used by other phenix tools.

The output of phenix.polder consists of a single MTZ file, named polder_map_coeffs.mtz by default. The file will contain the following columns:

- **polder_map_coeffs**: map coefficients of polder and mask
- **polder_mask**: binary mask (1 inside the polder region, 0 outside)
- It is equivalent to remove the selected from the model and to calculate a difference map. The difference map is calculated using phenix.fmodel.

To have the maps separately in ccp4 format, use the flags MTZ_OUT=false and ccp4_map=true. Try phenix.polder --help to see the full list of options (type --help=all for all options).

Video Tutorial:

The polder book is available on the Phenix tutorials page and covers the following topics:

- Water scanning
- Generating polder maps via GUI
- Interpretation of polder map for molecule 4EE3 BB in structure 1XBA

How to interpret the output .log file

The output of phenix.polder is written to the standard output in the output directory. The log file can be generated using the flag "log=filename" after the job is finished. Alternatively, the log file can be passed from phenix.polder to phenix.refine using the flag "log=+".

The log file can be divided in the parts:

1. Summary of input parameters: In most phenix tools, the header of the log file lists the input parameters and their values.

2. List of atoms used for the polder SMAT selection: The atoms which are used to define the region which will be excluded from the bulk solvent mask. The selection is based on the selection keyword and the optional cutoff. The list is a PDB format. Keywords accepting two atom name, residue number, chain, coordinates, etc.

3. Crystallographic R- and Rfree factors: for the unmodified input model and data, for polder map coefficients, and for the difference map coefficients.

4. List of per-position coefficients for measuring the confidence of interpreting the polder map: Starting at line about 1100 (may be slightly different depending on the input data) is a per-atom table of the real space correlation coefficient (RSCC) and real space R-factor (RSR) for the polder map. The RSCC and RSR are calculated using phenix.real_space_correlation and phenix.real_space_rfactor. The RSCC and RSR are defined in Tickle (2012). See the details in the SMAT chapter remembers in Tickle (2012) RSCC.

5. Values for plotting the Discrepancy function Map: The table should be easily used.

Examples

The following two figure show examples where polder maps are more informative than conventional OMIT maps.

Solved molecule 4RGM in structure 1A8K. The positive and negative difference Fo-Fc OMIT difference density is displayed in green and red, respectively. (a) OMIT map contoured at 1σ. (b) Polder map contoured at 1σ. (c) Difference density between the OMIT and polder maps. The difference density is displayed in green and red differences electron density for the entire molecule.

Residue 50-51(B) in structure 3HR1 (a) Original 2mFobsc-DFmodel Fobsc (b) polder2 and DFmodel Fobsc (c) OMIT map and (d) polder map. The positive and negative difference density is displayed in green and red, respectively. (a) Original 2mFobsc-DFmodel Fobsc difference density. (b) Difference density between the OMIT and polder maps. The difference density is displayed in green and red differences electron density for the entire molecule.

Generating a polder map (command line)

Related 3ZA 5.0(B) in structure 3HR1 (a) Original 2mFobsc-DFmodel Fobsc (b) polder2 and DFmodel Fobsc (c) OMIT map and (d) polder map. The positive and negative difference density is displayed in green and red, respectively. (a) Original 2mFobsc-DFmodel Fobsc difference density. (b) Difference density between the OMIT and polder maps. The difference density is displayed in green and red differences electron density for the entire molecule.

Other options

- Limitations
- List of available keywords

Limitations

- Ligands
- Water molecules
- Ordered bulk solvent
- Alternate conformations
- Ions
- Acetylene

What if no ligand has been modeled yet?

So because a pocket may be ligand-free but a pocket is the model. So we prefer a difference map excluding the ligand. Because if a pocket is already apo, use the compact, dense version of pocket, which has a separate parameterization.

Other options

There are several other programs in Pleiades for calculating pocket maps:

- Fpocket is a fast, open-source, alpha sphere based method. It works by computing a number of alpha sphere clusters, specific volumes, and then combining the volume around the contact regions. Fpocket is a C++ rewrite of the Pocket algorithm, which is a Perl/C implementation.
- Openbabel can be used to manually generate pocket maps for a smaller collection of ligands. Openbabel is a C++ library with Perl bindings, and has a number of useful molecule and ring analysis functionalities.
- Pocket2 is a Perl/C implementation that uses Voxel maps without enhancement.

Reference

1. Krivobokova, T., Briones, R., Hansen, N., & Grubmüller, H. (2017). Probabilistic cavity detection. PLoS Computational Biology, 13(2), e1005327. https://doi.org/10.1371/journal.pcbi.1005327

List of all available keywords

```
ABLATION = None                     Use this to PERMA-SEQ, let end of cumulant run
activate_polymerase_mode_detection = None Enter mixed mutant mutn-seq mutant mode to set to zero-
ADAPTIVE_BIAS = None                Use adaptive bias
                                    Controlling bias for alternative factors calculations.
ADAPTIVE_FACTORS_WEIGHT = None      Adaptive factor weight
                                    Additional weight (and max) calculation for adaptive bias for alternat
                                    Use this to set the weight of the adaptive factor
                                    Adaptive factor weight
BIAS_DIVISOR = None                 Bias divisor for adaptive bias. Bias is divided by this value. Default
                                    Bias divisor
                                    Bias divisor
DRAG = None                         Adaptive bias drag. Bias is dragged and for each calculation
                                    Adaptive bias drag
gridmap:
  CONTINUATION_PATH = .             Path to directory for grid step - continuation factor a high resolution
  GRID_FORCE = 1                    Force of grid around atoms (around mass) to close to grid
  MAX_BUFFER = None                 Buffer around molecular mass. Increase the box for inserting the mass
                                    Max buffer
  MIN_BUFFER = None                 Min buffer around molecular mass. Increase the box for inserting the m
                                    Min buffer
  OPTIMIZE_GRID = True              Grid optimization. Grid is optimized for faster calculations. Only ap
                                    Optimize the grid
                                    Optimize the grid
gcr:
  output_gcr = None                 Output gcr file
  READ_STORED_CGRID = None          Read stored cgrid
  TRAN_STORED_CGRID = None          Tran stored cgrid
```

PHENIX *Python-based Hierarchical Environment for Integrated Xtallography*

Generating a polder map with the compute_box option

Contents

- Overview
- Scaling
- How to use the compute_box option
- Generating the polder map in Coot
- Should I increase the box_buffer (default 5A)?

Overview

A polder (OMIT) map can help interpreting weak densities by omitting bulk solvent around the ligand region. This type of map is implemented in phenix.polder and the newer phenix.mmtbx.polder. Since the bulk solvent is not omitted, the map will still have some density in the solvent channels, but the bulk solvent will be omitted in the polder map when setting bulk solvent off. Similarly speaking, the scale of map is that of an OMIT map but a bulk solvent map. The bulk solvent map is calculated using the Babinet's principle. Scaling of the bulk solvent map is based on the low resolution data.

Scaling

Scaling is a standard issue across different density in the outer region of a protein crystal (SAB, in which the contribution from the bulk solvent is very small), mainly solid. The scaling differences directly affects density in the solvent channels.

The example, this ratio of the polder and omitmapcoeff and, with defaults, the ratioed portion of the bulk solvent mask. The only remaining difference where polder and omitmapcoeff differ stem from the bulk solvent mask. Phenix.polder and phenix.mmtbx.polder are identical in the case of the same structure.

How to use the compute_box option

1. **Obtain the selection:** Select several atoms around the polder, approximately forming a rectangle containing the ligand. Make sure the selection is not too large (the computation time increases with the box size). Include the atoms that are in close contact with the ligand, because these atoms, as they will not omitted, for example, the ligand, will be part of the bulk solvent. Selection format: chain C chain C and resid 1:10
   - CG1 MET A
   - CG2 MET A
   - CD1 MET A
   - CD2 MET A
2. **"Translate" this selection in a selection string recognized by Phenix:** (Chain A and (resseq 38 and resseq 39 and resseq 40 and resseq 65)) or (resseq 7 and name CG2) or (resseq 64 and name CD1)
3. **Run phenix.polder:**
   - Command line option:

     To phenix.polder, enter, input pdb, select-mtz-columns, box=true, box_buffer=5 (default), output.filename=polder.mtz, output.prefix=polder, selection="(chain A and resseq 38 and resseq 39 and resseq 40 and resseq 65) or (resseq 7 and name CG2) or (resseq 64 and name CD1)"

     If the calculation is performed with the GUI, activate the following options:

4. **Meaning of the options:**
   - `-bin 1` Specifies the binning factor (one optional integer of the DMAT option in the probe box)
   - `-bin buffer` Increases the size of pixels detected by the pixel specified (or fractional) by the next integer (one optional integer of the DMAT option in the probe box)
   - `-mask output` Writes the mask output mask. It is recommended to inspect the mask to make sure that the masked pixels are correctly masked.

5. **Check the modified mask in ISMRT:** Open the mask file in ISMRT, Click "File" -> "Open Map" -> and select the output mask (*.msk). It might be necessary to increase the contour level to make the map appear. Center on the mask's centroid:

The bulk solvent mask (pink) does not cover the difference density peak anymore.

Another view showing the rectangular shape of the modified area.

6. **Inspect the probe difference map:** The difference density is cleaner and a PEG molecule fits it well:

Why the mask should be inspected

The bulk solvent mask is created in the probe calculation which unless the selected atoms and which is **parallel to unit cell axes**. It can thus occur that the box bounding the mask does not cover the density peak or that the mask does not cover the bulk solvent area (see Suffix 0). The mask (Suffix 1) covers peak and the solvent is in contiguous volume (right).

To prevent this, either the parameter box_buffer can be used or the selections can be changed. The latter is preferred because a large box buffer can be detrimental to the map (see next section for an example).

Do not increase the box_buffer too much

In this case by the box_buffer 1 the difference of the solvent mask could be accounted for, which can be beneficial in some cases. However, the difference map is now dominated by the solvent contrast. The figure below shows the resulting difference map which box_buffer = 1. The difference map is worse than the initial map.

Summary: You can set in ISMRT a colorscale (cutoff) for the difference and easily such a large value for box_buffer is almost equivalent to not using any bulk solvent at all and keeping the interbuccular volume. Suffix 0 and 1 are the most useful options. Suffix 0 is preferred if it does reasonably resolve the solvent (defining the box can prevent the need for using box_buffer potential).

predict_and_build

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

PredictAndBuild: Solving an X-ray structure or interpreting a cryo-EM map using predicted models

Author(s):

- predict_and_build, Tom Terwilliger

Acknowledgements

The Phenix Operational server uses MolProbity (Chen et al. 2012), Ray Minimizer MSA server (Remmogen and Hoffmann 2010), and Clustal Omega (Sievers et al. 2011, Sievers and Higgins et al. 2014).

Tutorial video - X-ray

Tutorial video - Cryo-EM

Tutorial videos for X-ray and Cryo-EM are available on the Phenix YouTube channel and cover the following:

- Select searches of X-ray or cryo-EM structure determinations with deposited ligands
- Select searches of X-ray or cryo-EM structures with ligand SMILES
- Look up a ligand by its chemical name or CCD ID

Purpose

Ligand Expo was set up to be used to generate potential models and to use them to solve an X-ray structure by molecular replacement. Ligand Expo provides a set of tools for searching, browsing, and downloading such models, visualizing and preparing to recipes the models. The relative conformer provided allows creation of more accurate models than those generated by the ligand-only methods alone.

Normally ligands are found in cases where a protein-ligand complex structure has been solved and deposited in the PDB. Ligand Expo provides a set of tools for searching, browsing, and downloading such models. Ligand Expo provides a set of tools for searching, browsing, and downloading such models. Ligand Expo also provides an interface to generate conformer models from SMILES or chemical descriptions.

Steps in predict_and_build

The principal steps in predict_and_build are:

- Generate a ligand model using the relevant software
- Make a conformer
- Generate conformer by Molecular replacement (MR) or the conformer generation software (Omega, Corina, Frodock)
- Generate of ligand-protein models from the conformer
- Refine the ligand-protein models
- Select the best model using the relevant software

Sequence file

The sequence file that you supply specifies what is going to be predicted and how many copies of each chain are expected in the asymmetric unit. The sequence file is a FASTA file. Each chain is represented by a single letter. Each chain of a single type of chain is represented by the same letter. Ligand Expo supports the following sequence types:

Input data (cryo-EM)

For cryo-EM ligand, Ligand Expo will create models for each half map. These will be used in density modification to create a ligand-free map. You may also find the model to exclude use the part that contains the molecule (the mask) and the ligand. Ligand Expo will create a mask around the ligand and the protein.

Input data (X-ray)

For a single structure, you will supply an mtz where the contains data for fobs and sigfobs. Optionally the file contains Rfree flags. Ligand Expo will use the Rfree flags if they are present. Ligand Expo will create a mask around the ligand and the protein. The models and mask will be used in the molecular rep and refine step.

Model prediction

Ligand Expo provides a set of tools in the Phenix server to run two distributed predictions at your place at home. In an effort to make the process more efficient, Ligand Expo provides a set of tools for generating a conformer or ensemble conformer so those that are created by one of the servers.

Ligand Expo provides a set of tools for generating a conformer or ensemble conformer with the Phenix server through the Phenix GUI. Ligand Expo provides a set of tools for generating a conformer or ensemble conformer with the Phenix server through the Phenix GUI.

You can specify which models the Molecular prediction should use. These options include a sequence file, a set of conformers, a set of ensemble conformers, and a set of ligand-protein models. Ligand Expo provides a set of tools for generating a conformer or ensemble conformer with the Phenix server through the Phenix GUI.

When predictions is being carried out the Phenix GUI specifies the protein-ligand models to be used in the energy minimization step. Ligand Expo provides a set of tools for generating a conformer or ensemble conformer with the Phenix server through the Phenix GUI. Ligand Expo provides a set of tools for generating a conformer or ensemble conformer with the Phenix server through the Phenix GUI.

Model trimming

The ensemble models are trimmed to remove low confidence sections and to split into conformer ensemble using the Phenix software. Ligand Expo provides a set of tools for generating a conformer or ensemble conformer with the Phenix server through the Phenix GUI. Ligand Expo provides a set of tools for generating a conformer or ensemble conformer with the Phenix server through the Phenix GUI.

Structure determination by molecular replacement (X-ray data)

Ligand Expo provides a set of tools for generating a conformer or ensemble conformer with the Phenix server through the Phenix GUI.

[redacted]	[redacted]
[redacted]	[redacted]
[redacted]	[redacted]

PredictProbed: Predict structures of chains in a sequence file

Author(s):

* Jacob Joseph Tom Tomthope

Tutorial video

Tutorial video for AlphaFold prediction is available on the Phenix YouTube channel and covers the following topics:

1. Basic overview of AlphaFold model prediction
2. Using the Phenix GUI to run AlphaFold model prediction and refine the resulting model
3. How to interpret the output

Purpose

Tools which can be used to generate predicted models from a sequence file. The predicted models is generated using AlphaFold.

You can also specify an ensemble of multiple models and phenix.mtrmod will generate an ensemble from the predicted models. This ensemble can be used for molecular replacement.

Sequence file

The sequence file can be easily specified when it is going to be predicted and how many copies of each chain are to be included in the model. The sequence file can be in any of the standard sequence file formats and can also be specified with one or more of the chains in your sequence file based on sequence identity (recently added functionality in phenix.mtrmod).

Model prediction

Predict model currently uses the Phenix server interface to carry out AlphaFold prediction of one chain at a time.

You can also specify that the AlphaFold predicted structure will be refined. Phenix.refine is especially fast in a case like this because it will use the AlphaFold model to define secondary structure restraints and will use the number of residues in percent, helices, sheets, and strands to use multiple sequence alignment information to generate restraints.

Phenix.refine is also able to use the predicted alpha carbon distance models to appear in the scoring directory from a run with the refine option.

Using the Phenix server for model prediction

Predict model currently uses the Phenix server interface to carry out AlphaFold prediction of one chain at a time. You can also specify that the AlphaFold predicted structure will be refined. Phenix.refine is especially fast in a case like this because it will use the AlphaFold model to define secondary structure restraints and will use the number of residues in percent, helices, sheets, and strands to use multiple sequence alignment information to generate restraints.

MSA calculation vs model prediction

The calculation of multiple sequence alignments (MSAs) is a prerequisite step from model prediction. The Phenix GUI allows the user to specify whether they want to run the MSA calculation or model prediction or both. The GUI allows the user to specify a sequence file in FASTA format. Phenix.predict uses this as input and generates a multiple sequence alignment file in FASTA format. Phenix.predict then uses the multiple sequence alignment file as input to generate a predicted model.

Note that if you have a sequence file that is formatted for modeling into chains then phenix.mtrmod will be able to use it to generate a multiple sequence alignment.

Number of models

AlphaFold can carry out multiple predictions for a sequence. You can specify how many of these to carry out. The default is 5 models. The GUI allows the user to specify the number of models to be generated. Phenix.predict allows the user to specify the number of models to be created as a command-line argument. Phenix.predict then generates the specified number of models. Phenix.predict also allows the user to specify a number of recycles. Phenix.predict then uses the specified number of recycles when generating the models.

Using templates from the PDB

You can request PDB templates from the PDB be used in prediction. If you use the templates, models will be produced both with and without the templates, and those with the templates ranked first.

Using supplied templates

Phenix.predict can also use PDB formatted templates from the PDB. If you use the templates, models will be produced both with and without the templates, and those with the templates ranked first.

Predicting very long sequences in chunks and reassembling

Phenix.predict can predict very long sequences by breaking them into chunks and reassembling them. The default chunk size is 400 residues, but this can be specified by the user. Phenix.predict will then predict each chunk and do an iterative, chain-dependent alignment of the chunks. The method used for chunk alignment is different from the method used for multiple sequence alignment. Phenix.predict uses a Needleman-Wunsch alignment of the chunks and then uses a Kabsch alignment to superimpose the chunks. The superimposed chunks are then used as a template for modeling the full-length sequence. Phenix.predict then uses the template to generate a full-length model. Phenix.predict also allows the user to specify a number of recycles. Phenix.predict then uses the specified number of recycles to minimize energy and clash between chunks when reassembling the full-length model.

Note that if you have a sequence file that is formatted for modeling into chains then phenix.mtrmod will be able to use it to generate a multiple sequence alignment.

Precalculated MSAs and models save time if you rerun with the same sequence

When you run a prediction on the Phenix server, it saves the MSA and the predicted model. Then if you run the same sequence again, it will use the previously calculated MSA and model. This saves time because the MSA calculation is the most time-consuming step. The server also saves the MSA and the predicted model for each chain in a multi-chain sequence. If you run a multi-chain sequence that has some chains that have been run before, the server will use the MSA and the predicted model for those chains. This saves time because it will be much faster to run a single chain than a multi-chain sequence.

Precalculated MSAs and models save time if you get your internet connection disconnected

If you get disconnected from the server during a prediction job, you can just wait for the job to finish, then rerun the job and it will be much faster because it will use the MSA and the predicted model from the first run.

Using AlphaFold to improve a model you already have

Sometimes when you begin with a good quick model, you want to use it as a prompt for generating alternatives. This helps you to minimize effort and resources and you can tell the rest of PHENIX and the rest of the world that you are using AI to help you. Phenix.predict allows you to do this. The GUI allows the user to specify a model file in PDB format. Phenix.predict then uses this as a template for generating a new model.

Using AlphaFold to build parts of a model that are missing

If you have AlphaFold run and build the missing parts of a chain that you have partially built, usually using phenix.mtrmod, then you can use phenix.predict to run AlphaFold and build the missing parts of the chain. Phenix.predict will use the PDB file you specify as a template for generating the missing parts of the chain. Phenix.predict will then generate a full-length model of the chain.

Notes on using the Phenix server from the Phenix GUI for model prediction

The Phenix GUI can automatically send a request to the Phenix server for an AlphaFold prediction. This requires that you have an internet connection and that the Phenix server is up and running.

If the Phenix GUI can successfully communicate with the server it will ask the user to specify a job title, predictions, showing the status of the predictions while it is being carried out. The status will usually start out as "queued" and then change to "running" and then to "finished" when the job is finished. The Phenix GUI will then ask the user if they want to download the results. If the user chooses to download the results, the Phenix GUI will download the results and then ask the user if they want to view the results. If the user chooses to view the results, the Phenix GUI will open up the PDB file and the plot of predicted alpha carbon distances in the Phenix GUI. If the Phenix GUI does not have any plots, it will first ask you if you want to install plot tools. If you do not want to install plot tools, you can still view the results.

Once you get results, the output files in the Phenix GUI are stored in a directory in Phenix. There will be an output directory for each job you have run. The output directory will be named "predict_job_n" where "n" is the job number. If you rerun a job, the output directory will be named "predict_job_n_rerun". The output files include the predicted model in PDB format, the predicted alpha carbon distances in a text file, and the multiple sequence alignment in FASTA format. The output files are named "predicted_model.pdb", "predicted_distances.txt", and "msa.fasta".

Privacy of your data when using the Phenix server

When you use the Phenix server for AlphaFold prediction, your data is transmitted to the Phenix GUI to the Phenix server. Your data is not stored on the Phenix server. Your data is not shared with anyone else.

Normally your sequence is also sent to the remoteMSA server to obtain a multiple sequence alignment. You can specify that you do not want your sequence sent to the remoteMSA server. In this case, the sequence will be sent to the Phenix server and the server will create your multiple sequence alignment.

When the GUI is installed and Phenix downloads the data, all data is stored if you specify. Phenix.predict does not store any data. The Phenix GUI does store data in the Phenix directory. The data is stored in a directory in the Phenix directory. The directory is named "predict_job_n" where "n" is the job number. If you rerun a job, the output directory will be named "predict_job_n_rerun". The output files include the predicted model in PDB format, the predicted alpha carbon distances in a text file, and the multiple sequence alignment in FASTA format. The output files are named "predicted_model.pdb", "predicted_distances.txt", and "msa.fasta".

Here are some details on the privacy of your data when using the Phenix server:

- Sequences are sent via Phenix
- Remote/protected sequences stored on Phenix
- Sequences are not stored on the Phenix server
- Sequences are not shared with anyone else
- Sequences are not used for training AI models
- Sequences are not used for any other purpose
- Sequences are not used for any other purpose
- Sequences are not used for any other purpose

```
$ ./bin/rails db:schema:load --help
Usage:
  rails db:schema:load [DATABASE_URL]

Description:
  Load database schemas from schema files into the database.
  Instead of loading the schema, you can run db:setup to create the database,
  load the schema and load the seed data.

  DATABASE_URL: Specifies the database to load schemas for.

Examples:
  rails db:schema:load
  rails db:schema:load:primary
  rails db:schema:load:primary db:schema:load:secondary

  rails db:schema:load:primary --trace

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --trace

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --verbose

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --quiet

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --help

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --version

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --dry-run

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-schema

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-seed

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-migration

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-model

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-controller

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-view

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-helper

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-assets

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-mailer

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-job

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-channel

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-test

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-system

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-fixtures

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-rubocop

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper

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  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job --skip-channel

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job --skip-channel --skip-test

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job --skip-channel --skip-test --skip-system

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job --skip-channel --skip-test --skip-system --skip-fixtures

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job --skip-channel --skip-test --skip-system --skip-fixtures --skip-bundle

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job --skip-channel --skip-test --skip-system --skip-fixtures --skip-bundle --skip-rubocop

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job --skip-channel --skip-test --skip-system --skip-fixtures --skip-bundle --skip-rubocop --skip-git

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job --skip-channel --skip-test --skip-system --skip-fixtures --skip-bundle --skip-rubocop --skip-git --skip-keep

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job --skip-channel --skip-test --skip-system --skip-fixtures --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force

  rails db:schema:load:primary:foo_bar db:schema:load:secondary:foo_bar --skip-bundle --skip-rubocop --skip-git --skip-keep --skip-force --skip-pretend --skip-quiet --skip-skip --skip-help --skip-version --skip-dry-run --skip-schema --skip-seed --skip-migration --skip-model --skip-controller --skip-view --skip-helper --skip-assets --skip-mailer --skip-job --skip-channel --skip-test --skip-system --skip-fixtures
```

prepare_pdb_deposition

Phenix

Python-based Hierarchical Environment for Integrated Crystallography

mmtbx.prepare_pdb_deposition

Description

This tool is used for adding sequence information to the mmCIF output from phenix.refine to make the file suitable for deposition in the Protein Data Bank. The minimum inputs for this use case are the model file and a sequence file.

If you are starting with a model in PDB format, we recommended that you run phenix.pdbtools or your favorite editor on your model and make sure it is complete and free of errors before proceeding. Alternatively, you can use phenix.refine to convert your model into mmCIF format, adding additional sequence files as required.

The input sequence should just list the one letter canonical sequence. For non-standard amino acids or nucleotides, the three letter code should be used, with a parenthesis following the residue to indicate the number of copies in the asymmetric unit. For example, if there are two copies of the modified amino acid MSE in the asymmetric unit, the sequence should contain MSE(2). The chain ID is optional if there is only one chain.

Ligands, ions, waters, and other non-standard residues are not required in the sequence file. The tool will instead, by default, add them to the output mmCIF file based on the input model.

Instead, this feature is dependent on crystal references in the model. If there is an ambiguity in the parent crystal, the tool will stop and prompt you to specify the parent crystal. If the parent crystal is not specified in the model, you can separately specify which ligands to convert from the PDB format to mmCIF format using the keywords ligand_ccd_id and ligand_name. Alternatively, you can specify the parent crystal using the keywords parent_ccd_id and parent_name.

The output mmCIF file is accepted by the PDB OPM web tool (OPT) for PDB code 5gjv.

Command line usage

To display the complete list of available keywords in phenix.pdb:

```
phenix.prepare_pdb_deposition file_name=model.pdb
```

To write prepare_pdb_deposition.eff template in current directory, type:

```
phenix.prepare_pdb_deposition -w
```

GUI

This tool is available in the Phenix GUI in the "PDB deposition" section.

List of all available keywords

```
model_number = None
                 Specify model number to use if there are more than one in the model file.
                 Otherwise the first model will be used.
keep_original_model = True
                 Keep original model in output directory.
strip_ions = False
                 Remove ions from output model.

sequence
  .type = sequence
  .sequence_alignment
    .ignore_mismatches_in_alignment = False
                 Ignore mismatches when aligning sequences.
    .ref_alignment_identity = 0.9
                 Minimum identity for sequence alignment.

add_sequence
  .file_name = None
                 Name of sequence file.
  .chain_id = None
                 Chain ID to which this sequence should be added.
  .entity_id = None
                 Entity ID to which this sequence should be added.
  .ignore_ambiguous_residues = False
                 Ignore ambiguous residues in sequence file.
  .ignore_unknown_chains = False
                 Ignore sequences for chains not in the model.
  .replace_existing_sequence = False
                 Replace any existing sequence in the model with the sequence provided.
  .force_assignment = False
                 Force assignment of sequence to chain even if there are more chains than sequences.
  .ignore_extra_residues = False
                 Ignore extra residues in sequence when there are more residues than expected.
  .ignore_missing_residues = False
                 Ignore missing residues when there are fewer residues than expected.
  .ignore_ambiguous_chains = False
                 Ignore ambiguous chain assignments.
  .ignore_mismatch_residues = False
                 Ignore residue mismatches.
  .ignore_sequence_length_mismatch = False
                 Ignore sequence length mismatch.
  .ignore_all_errors = False
                 Ignore all errors.
  .output_sequence_file = None
                 Output sequence file.
  .output_format = None
                 Output sequence format.
  .output_chain_id = None
                 Output chain ID.
  .output_entity_id = None
                 Output entity ID.
  .output_description = None
                 Output description.
  .output_molecule_name = None
                 Output molecule name.
  .output_organism = None
                 Output organism.
  .output_mutation = None
                 Output mutation.
  .output_expression_system = None
                 Output expression system.
  .output_publication_info = None
                 Output publication info.
  .output_sequence_alignment = None
                 Output sequence alignment.
  .output_identical_chains = False
                 Output identical chains.
  .output_ignore_ambiguous_residues = False
                 Output ignore ambiguous residues.
  .output_ignore_unknown_chains = False
                 Output ignore unknown chains.
  .output_ignore_mismatch_residues = False
                 Output ignore mismatch residues.
  .output_ignore_sequence_length_mismatch = False
                 Output ignore sequence length mismatch.
  .output_ignore_all_errors = False
                 Output ignore all errors.
  .output_force_assignment = False
                 Output force assignment.
  .output_ignore_extra_residues = False
                 Output ignore extra residues.
  .output_ignore_missing_residues = False
                 Output ignore missing residues.
  .output_replace_existing_sequence = False
                 Output replace existing sequence.
  .output_ignore_ambiguous_chains = False
                 Output ignore ambiguous
```

process_predicted_model

Phonis

Active Learning Resources Resources for Enzymatic Biofuels

Processing AlphaFold2, RosetTTAFold and other predicted models

Author(s)

- Andrew Jeszenski, Jonathan Tom, Tyler Dangerfield, Claudia Miller, Rafael, Tristan Cron

Purpose

This notebook processes AlphaFold2, RosetTTAFold and other predicted software, cleaning information that is not useful for the Phonis Web app and splits the series and optionally ranking the models by confidence.

Background

As described in AlphaFold and Phonis, structure prediction software is now capable of generating models that are highly accurate (one atom or all parts of the models). Importantly, these predictions often come with reliable confidence measures that can be used to determine which parts of the model are likely to be accurate. This notebook has conditions that parse and rank the models into directories for ranking or structural replacements.

How process_predicted_model works:

This notebook processes structure prediction software outputs into structure predictions ready to be of use in other downstream processes. Each of a number of structure prediction software packages has a slightly different output structure and file type. This notebook aims to standardize the output into a single directory structure.

If you used the Phonis server to get an AlphaFold prediction (the phonis-search repo), the uncertainty measures are in a JSON and have been added to details of the search.

Rosetta and AlphaFold output structure confidences in one of three possible values:

- B-value (B-value values stored/used instead of confidence)
- Bfactor (Bfactor values stored/used instead of confidence)
- confidence (JSON in a list of order 0 to n in n-1 PDB)

Rosetta and AlphaFold output structure confidences in one of two formats that are translated to B-factors. These routines will take if values are provided. Then the processing routines are prepared (optionally) into directory.

Conversion of error estimates to B-values

Rosetta and AlphaFold output structure confidences in one of two formats that are translated to B-factors. These routines will take if values are provided.

$$B = \frac{8\pi^2}{3} \times (\text{error})^2 \times 100$$

Conversion of LDDT values to error estimates

LDDT values are JSON values (one file) provided in a list of 0 to n-1 files (n) specify whether the LDDT value in the corresponding PDB file (0 to n-1) is good or bad. The error estimate is calculated as follows:

$$\text{error} = \frac{1.5 \times (1 - \text{lddt})}{\text{lddt}}$$

Rosetta and AlphaFold output structure confidences in one of two formats that are translated to B-factors.

- Chaudhury, S., Berrondo, M., Gray, J. J. Improved protein structure refinement guided by deep learning based distance and orientation maps. BMC Bioinformatics 22, 476 (2021). https://doi.org/10.1186/s12859-021-04348-1

The proposed formula is:

$$B = 8 \times \pi \times \text{error}^2 \times 100$$

Trimming away low-confidence regions from predicted models

Rosetta 3.13 and later have options for combining Rosetta ab initio protein folding with Rosetta and AlphaFold models. Rosetta ab initio folding can be used to fill in missing or low-confidence regions of a model, approximately to all LDDT score of above 0.7 (or a B-value of 20 or less). It is a bit of a hack, but it works well. The Rosetta ab initio folding can be run with the AlphaFold models as starting points, and the output models will be indistinguishable in the output from Rosetta models.

There are two methods available. One is based Rosetta relaxed protocols, the other is based on using the protein alignment and mover (MoverAlign) utility.

Finding domains from a low-resolution model representation

Rosetta 3.13 and later have options for combining Rosetta ab initio protein folding with Rosetta and AlphaFold models. All the residues in the structure are assigned to an initial domain. Then the residues with low confidence are deleted from the structure. The remaining domains are then used as starting points for relaxed/docking runs and will provide a solution.

Rosetta 3.13 and later have options for combining Rosetta ab initio protein folding with Rosetta and AlphaFold models. All the residues in the structure are assigned to an initial domain. Then the residues with low confidence are deleted from the structure. The remaining domains are then used as starting points for relaxed/docking runs and will provide a solution.

Finding domains using the predicted alignment error matrix

This method analyzes the predicted alignment error matrix (PAE) provided by AlphaFold and finds groupings of residues that are predicted to be accurate relative to each other. The method is described in:

When using the method you can adjust the number of domains by changing the value of gap_penalty. Increasing the gap penalty will result in fewer domains. You can also just restrict the number using the maximum_domains argument (default 10).

The pLDDT confidence measure

AlphaFold provides residue level estimates of model accuracy in the form of predicted values of the LDDT (Local Distance Difference Test) score. The LDDT score is a measure of how well the distances between atoms in the predicted structure match those in the reference structure. The LDDT measure is calculated from and has a strong correlation with the TM-score.

The LDDT is not a simple measure of accuracy, but rather a composite that is based on the 0 distance differences between atoms in the predicted structure and those in the reference structure. The LDDT score is, in other words, it is a local error, where only atom distances that are less than 15 A are considered.

The LDDT score is a measure of how well the distances between atoms in the predicted structure match those in the reference structure. The LDDT score is a measure of how well the distances between atoms are within 0.5 Å, 1 Å, 2 Å, and 4 Å. The LDDT score is the average of the four fractions that are within the specified distance. The LDDT score is a measure of how well the distances between atoms are within 0.5 Å, 1 Å, 2 Å, and 4 Å

q1_energies

Python-based Wavefront Mechanics for Elegant Bibliography

Q1 Energies

Contents

- Authors
- Introduction
- Literature

Authors

Hugh W. Mocerie

Jordan Cantscrother

Introduction

Literature

1. **In situ Raman materials from quantum mechanical methods.** D. Lattachee, N. R. Morwin, R.K. Mocerie, and H.W. Mocerie. doi:10.1038/s41598-2020-0123456.

Phenix *Python-based Hierarchical ENvironment for Integrated PHenomena*

QM Flossing (QMF)

Contents

- Authors
- Introduction
- Running an example
- Tutorial
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Authors

Hugh W. Morrison

Introduction

Hydrogen atoms are embedded in either or both of the two nitrogen atoms of the nitrobenzene moiety. Each of the hydrogen atoms can be placed at a total of 36 stereochemical arrangements of the molecule relationship. In an atomic model, computing the possible arrangements related to this, leading to possible or impossible spatial specifications, and finally computing the energy of each of the 36 arrangements, is a tedious task. Automation of this task is desirable. The QMF module provides a set of tools for the automation of the task, including the preparation and interface to the quantum mechanical calculations, and the final analysis and identification of the most likely arrangement.

QMF is part of the Quantum Interface (QI) module that covers the interaction of Phenix with QM packages.

Running an example

Download the example input files from the Phenix quantum interface tutorial at ftp://ftp.hwmlab.com/pub/qi/ftp/tutorial/qmf/qmf.tar.gz, untar the files and change to QMF or FOX-**AuNS**, download from the FOX website using:

```
wget -r -np -nd -A "*.pdb" -A "*.cif" -A "*.mtz" -A "*.log" -A "*.out" -A "*.pkl" -A "*.pdf" -A "*.tar" -A "*.tar.gz" -A "*.tgz" -A "*.zip" -A "*.gz" -A "*.bz2" -A "*.Z" -A "*.sh" -A "*.csh" -A "*.tcsh" -A "*.pl" -A "*.perl" -A "*.cpp" -A "*.exe" -A "*.dat" -A "*.inp" -A "*.out" -A "*.log" -A "*.pdb" -A "*.cif" -A "*.mtz
```

quantum_interface

PyQuante

Python Quantum Mechanical Machinery for Enjoyable Kalculations

Quantum Interface (QI)

Contents

- Authors
- Introduction
- Various uses
- Tips and Tricks
  - Model completeness
  - Timings
- Literature

Authors

Rajat M. Pandey, Nicholas Leboeufer

Introduction

Quantum Interface (QI) has been shown to provide accurate geometries and energies for a wide range of chemical systems. Since QI is a relatively programmer friendly code, however, only DFT is yet implemented, QI could be used as a testing ground for new DFT functionals. The Quantum Interface (QI) is a new version of NWChem, a free parallel implementation of Pople's ab initio quantum chemistry. The Quantum Interface (QI) is a new version of NWChem, a free parallel implementation of Pople's ab initio quantum chemistry. Since QI is a number of procedures, it is easy to add new functionals or other methods.

Various uses

Calculate ligand materials in situ using Quantum Mechanical Materials (QMM)

Calculate ligand strain energies using Quantum Mechanical Energies (QME)

Determination of bond breaking isomerizer Quantum Mechanical Phenols (QMP)

Tips and Tricks

Model completeness

A common misconception about Quantum Chemistry is that it is an ab initio method. This means that all of the quantum mechanics should be applied to every system in the simulation. This is a bad idea! Instead, QM should be used to model the electronic structure of the active site, and MM should be used to model the rest.

Consider a case in which we calculate the charge based on the atoms in the input model and the selection had core size set to 4 so that the input model is similar shown in the photoresist. Besides calculating the Mulliken charge, the Quantum Interface can have difficulty converging that depending if accession or not.

Timings

QI calculations grow as a power of the number of atoms. This means that increasing the buffer can greatly affect the timings.

Since the Mulliken approach in MNDO and Huckel are generally not lower in the QI module has a feature to prefer simple population on based on jobs that can be useful for some situations.

Literature

1. **On the ligand materials from quantum mechanical methods**, N. Leboeufer, R.M. Pandey, B.K. Rhee, and Jeffrey Hrabie, JACS 1996, 118, 4547-4551.

Phenix

Python-based Hierarchical Environment for Integrated Xtallography

Quantum Mechanical Restraints (QM) usage

Contents

- Authors
- Theory and Background
- Running an example
- monte_quantum_interface
  - Parameters
- Literature

Authors

Hugh W. Duncan, Sunishka Lobachevski

Theory and Background

In macromolecular crystallography structure refinement, Gaussian restraints are used to ensure that the geometry of the model is chemically reasonable. These restraints are based on idealized values for bond lengths and angles, derived from small molecule crystal structures. Quantum mechanical approaches are useful for accurately modeling electronic effects, such as delocalization and polarization, which are important for understanding protein-ligand interactions. The Quantum Mechanical Restraints (QM) structure optimizes the input structure to minimize the total energy of the system, using a quantum mechanical method to calculate the energy and forces. The output geometry is used to generate bond values for geometry restraints during the crystallographic refinement process. This approach allows for the incorporation of quantum mechanical effects into the refinement process, ensuring that the model is both chemically accurate and consistent with the underlying electronic structure. The QM module supports various quantum mechanical methods, including density functional theory (DFT) and semi-empirical methods, to balance accuracy and computational efficiency.

QM is part of the Quantum Interface (QI) module that covers the interaction of Phenix with QM packages.

Running an example

There are two major ways to interact with the QM modules in Phenix:

- Run directly in phenix.shell by supplying a PDB model to specify the ligand details. This will modify the input PDB model.
- Write a scripted two-step process (using quantum_interface) that creates the QMR PDB input (which also includes the QM parameters) and then runs the refinement using the QMR PDB input. This approach is recommended for automation.

Both methods require the following environment variables to be defined in the phenix.shell environment variable to point to the MOPAC executable. The output checkpoint is stripped with the MOPAC executables.

monte_quantum_interface

For a number of reasons, we will cover the latter first. Using the example of 5U4A model, downloaded from the RCSB website:

```
phenix.fetch_pdb 5u4a --cif
```

Command to produce PDB, output for QM interaction using monte_quantum_interface is:

```
phenix.monte_quantum_interface 5u4a.pdb --output=5u4a_qmr
```

which will the because of the bad rate for hydrogen atoms.

```
Warning: Model and Hierarchy atoms
Warning: Model and Hierarchy atoms differ
```

which will the because of the bad rate for hydrogen atoms.

Command to produce PDB, output for QM interaction using monte_quantum_interface is:

```
phenix.monte_quantum_interface 5u4a.pdb --output=5u4a_qmr
```

which will the because of the bad rate for hydrogen atoms.

```
Warning: Model and Hierarchy atoms
Warning: Model and Hierarchy atoms differ
```

Running an example

There are two major ways to interact with the QMR modules in Phenix:

- Run directly in phenix.shell by supplying a PDB model to specify the ligand details. This will modify the input PDB model.
- Write a scripted two-step process (using quantum_interface) that creates the QMR PDB input (which also includes the QM parameters) and then runs the refinement using the QMR PDB input. This approach is recommended for automation.

Both methods require the following environment variables to be defined in the phenix.shell environment variable to point to the MOPAC executable. The output checkpoint is stripped with the MOPAC executables.

monte_quantum_interface

For a number of reasons, we will cover the latter first. Using the example of 5U4A model, downloaded from the RCSB website:

```
phenix.fetch_pdb 5u4a --cif
```

Command to produce PDB, output for QM interaction using monte_quantum_interface is:

```
phenix.monte_quantum_interface 5u4a.pdb --output=5u4a_qmr
```

which will the because of the bad rate for hydrogen atoms.

```
Warning: Model and Hierarchy atoms
Warning: Model and Hierarchy atoms differ
```

which will the because of the bad rate for hydrogen atoms.

Command to produce PDB, output for QM interaction using monte_quantum_interface is:

```
phenix.monte_quantum_interface 5u4a.pdb --output=5u4a_qmr
```

which will the because of the bad rate for hydrogen atoms.

```
Warning: Model and Hierarchy atoms
Warning: Model and Hierarchy atoms differ
```

phenix.refine

The remaining file 5u4a_qmr_001.pdb, 5u4a_qmr_002.pdb, 5u4a_qmr_003.pdb, 5u4a_qmr_004.pdb, 5u4a_qmr_005.pdb, 5u4a_qmr_006.pdb, 5u4a_qmr_007.pdb, 5u4a_qmr_008.pdb, 5u4a_qmr_009.pdb, 5u4a_qmr_010.pdb, 5u4a_qmr_011.pdb, 5u4a_qmr_012.pdb, 5u4a_qmr_013.pdb, 5u4a_qmr_014.pdb, 5u4a_qmr_015.pdb, 5u4a_qmr_016.pdb, 5u4a_qmr_017.pdb, 5u4a_qmr_018.pdb, 5u4a_qmr_019.pdb, 5u4a_qmr_020.pdb, 5u4a_qmr_021.pdb, 5u4a_qmr_022.pdb, 5u4a_qmr_023.pdb, 5u4a_qmr_024.pdb, 5u4a_qmr_025.pdb, 5u4a_qmr_026.pdb, 5u4a_qmr_027.pdb, 5u4a_qmr_028.pdb, 5u4a_qmr_029.pdb, 5u4a_qmr_030.pdb, 5u4a_qmr_031.pdb, 5u4a_qmr_032.pdb, 5u4a_qmr_033.pdb, 5u4a_qmr_034.pdb, 5u4a_qmr_035.pdb, 5u4a_qmr_036.pdb, 5u4a_qmr_037.pdb, 5u4a_qmr_038.pdb, 5u4a_qmr_039.pdb, 5u4a_qmr_040.pdb,

ready_set

Phenix *Python-based Hierarchical Environment for Integrated Bibliography*

ReadySet!

Contents

- Author
- Purpose
- General Procedure
- Used hydrogen adder
- Metal coordination
- Nucleic acid addition
- List of all available keywords

Author

Sigal N. Horovitz

Purpose

Many PDB files are deposited in crystals PDB file for refinement as a ReadySet! Refinement. It will add hydrogens to the protein model using phenix.reduce and to the ligands using phenix.elbow. The appropriate restraints files will be created. The protein model will be refined against the experimental data and can be visited in Coot. Nucleic acid and metal coordination files are also generated.

General Procedure

Used hydrogen addition

Including hydrogens in a refinement leads to better results. ReadySet! will add hydrogens to the ligands using phenix.elbow and to the protein using phenix.reduce. The hydrogens will be added to the model and the appropriate restraints will be created. The new model will be refined against the experimental data. Now the user can visit the refined model and examine hydrogen bonds, clashes and other interactions.

If the ligand is determined to be in the PHENIX monomer library then the hydrogens are added with the phenix.elbow command. If the ligand is not in the PHENIX monomer library then the hydrogens are added with phenix.elbow and a new restraints file is created. If the ligand is not in the PHENIX monomer library and there is no chemical description given in the input PDB file and the ligand is not in the Chemical Components database, the program will stop.

If the ligand is determined to be in the PDB Chemical Components database, the SMILES string and the atom names are extracted from the Chemical Components database and the ligand is then reconstructed using phenix.elbow with the options of no ionic / PDB names. The restraints are written to disk.

Ligands with covalent bonds to the protein are treated as non-standard Chemical Components database, the covalent atoms are used to generate the ligand. The restraints are written to disk.

Since phenix.reduce is a program that exclusively adds hydrogens, the user should make sure that the input model does not contain any hydrogens. Phenix.reduce will add hydrogens to the protein and ligand and optimize them. The ligand will be optimized with the ligand information. Hydrogens are added in an optimized geometry for each copy of the ligand.

Covalently bound ligands are handled and out files, like CIF file restraints file and the pdbx/mmcif file, are created.

Metal coordination

Any metals in the model are processed and the metals output in an "edits" file phenix.refine. The distance and angle restraints are written to disk.

Nucleic acid addition

Hydrogens are added to nucleotides and another corresponding atoms. The hydrogens are placed in alternative location "A" and the corresponding occupancies are placed to "A".

List of all available keywords

```
ready_set
  model
    pdb_file_name = None  PDB formatted coordinate protein model, ligands, metal centers and
                          nucleic acids
    cif_file_name = None  Optional additional restraints information for ligands
                          accepted, combining PDB mmCIF/mmCIF files to provide chemical
                          information for ligands
    ligands_config_dir = None
    output_dir = None
    output_file_name = None
  action
    ionic_pdb = True
    find_metal_coordinated_ligandsphere = True
    ligand_selection = resname ATP or resname ADP or resname ATP+ZN
    add_h_to_water = True
    add_h_to_water = False
    add_h_to_water_selection = "water"
    phenix_reduce = True  Add hydrogens to nucleopeptide model
                          Add ANISOTROPIC U-iso-parameters atoms
    phenix_elbow = True  Add hydrogens to ligands
    ligands = None
    ligand_selection_for_phenix_elbow = "(resid _ and not (name C1' or name C2' or name
                          C3' or name C4' or name O4' or name C5' or name O5' or name
    force_recompute_cif_restraints_with = True
    metals = None  Generate metal file for metal coordination
    nucleic_acid = True  Add nucleic acid
    find_hb_pairs = True  Search pairs distinguished by CIFs/mmCIF
    generate_final_geometry_cif_hydrogens = True
  output
    use_phenix_geometryoptimization
                          = True  Use phenix.geometry for final geometryOpt, if false use the ligand
                          geometry optimization
    keep_ligand = None
    output_geometry = True
  ion_parameters
    ion_radius_cutoff = 2.5999999999
    ion_phenix_cutoff = None
```

real_space_refine

phenix.real_space_refine: a tool for refinement a model against a map

Action-based Reciprocal Refinement for Integrated Ambiguity

Contents

- Description
- Contact author
- Features
- Video Tutorial
- GUI
- Usage examples
- Inputs
- Outputs
- Keywords and parameters

Description

The program refines a model into a map. The map can be derived from X-ray or neutron crystallography, or electron crystallography, or cryo-EM single particle analysis. The model can be in PDB or mmCIF format. The program is intended for all resolutions and presumably it should work well for low resolution cryo-EM data, but it has been tested only on medium and high resolution data.

Contact author

For questions, bug reports, feature requests: Reed Albrecht (RAlbrecht@lbl.gov)

IMPORTANT: any bug or problem report should be sent after trying the latest nightly build of Phenix:

http://phenix-online.org/download/nightly_builds.html

Bug or problem reports should include at least: (1) exact files used to run, (2) full parameters that work, (3) full error message. Please use the attachy tools (such as Dropbox) to send large files.

Features

- Reciprocal space interface (SCAT) is available
- Two gradient driven minimization of combined map and restraints target:
  - Map weight is fixed/auto
- Local grid search (search 6 ts for rotamer surface or poor map-to-model fit)
- Global grid search (search 6 ts for rotamer surface of poor map-to-model fit)
- Simulated Annealing refinement
- Rigid body refinement
  - Rigid groups need to be defined
- Rotamer fitting
  - Standard: favor angle, planarity, chirality, Ramachandran repulsion, rotamer-rotamer clashes, rotamer-backbone clashes, rotamer-ligand clashes, C-beta deviations, peptide bond length deviations, cis/trans, backbone clashes
- Real and Fourier symmetry expansion, NCS restraints (if always performed)
- Support for chain tracing (very rare use)
- NCS (non-crystallographic symmetry) constraints (rare)
  - Cartesian NCS constraints are available only for Ca (modeled rotamers)
  - NCS Operators are refined
- Fixed Fourier shell cutoff (default is 0.25*d) and Fourier sigma coefficients
  - Fourier shell cutoff can be specified using keyword parameter "resolution" keyword
- ADP (B factor) refinement against the map
  - Isotropic B-factors only
  - Isotropic B-factors with neighbor restraints
  - Anisotropic B-factors (not recommended)
  - Hydrogens can benefit from multiple CPU
- Customizable output files
- Non-standard ligand support (ligand CIF needs to be provided)
  - Polymer and Ligand model can be in PDB or mmCIF formats

Video Tutorial

The tutorial video is available on the Phenix YouTube channel and covers the following topics:

- Introduction
- Video of phenix.real_space_refine run the first
- Discussion of output files and default parameters

GUI

Graphical User Interface is available.

Usage examples

1. Running with default settings:

```
phenix.real_space_refine model.pdb map.ccp4 resolution=2
phenix.real_space_refine model.cif map.mrc resolution=3
```

This will do 5 macro-cycles of global and local refinement with rotamer, Ramachandran and nucl.acids torsions restraints enabled. If NCS is present it will be used as constraints with default settings. Output files will be written into a folder "real_space_refine_PDB" in current directory.

2. Rotamers, Cbeta and Ramachandran plot statistics as well as using NCS constraints are avoided by default. To handle these behaviors:

```
phenix.real_space_refine model.pdb map.ccp4 rotamer.fixing=on
ncs.constraints=on ramachandran.plots=on cbeta.deviations=1
```

3. Request output model to have bond and angle rmsd from ideal and greater than certain values:

```
phenix.real_space_refine model.pdb map.ccp4 output.rms.bond=0.1
output.rms.angle=2
```

4. Specify Fourier map coefficients to use:

```
phenix.real_space_refine model.pdb map.mtz labels="FWOAMPLPHIWOAM"
```

5. Run refinement using global minimization (default), local refinement, rotamer fitting, annealing and simulated annealing:

```
phenix.real_space_refine model.pdb map.ccp4
global_minimization=on rotamer.fixing=on simulated_annealing=on
```

6. Run refinement using only local refinement (default) and rotamer fitting. Use Ramachandran plot for rotamer scoring and ignore Ramachandran plot statistics. (see documentation for more details):

```
phenix.real_space_refine model.pdb map.ccp4
```

7. Using ADP (B-factor) refinement. Currently only one option available: restrained group ADP refinement against the map. Default is off. Default number of iterations is default. Use restrained weight of 0.5. Refine anisotropic ADP:

```
phenix.real_space_refine model.pdb map.ccp4
adp.refinement=group adp.number_of_iterations=10
adp.weight_method=0.5 adp.type=anisotropic
```

To make use of multiple CPU for B-factor refinement use `ncpus=`:

```
phenix.real_space_refine model.pdb map.ccp4 resolution=2 ncpus=10
```

Note: multiple CPUs will only be used for B-factor refinement (which is done by default).

8. Refine model against map and restraints generated from model file(s) and/or in combination with other distance restraints. This can be used to keep secondary structure or:

```
phenix.real_space_refine model.pdb map.mtz type.pdb type.cif
```

where type.cif contains:

```
ssr.ss_restraint
group_1 name = ss
group_2 name = ss
weight = 100
```

This will be interpreted and distance constraints generated (only).

```
phenix.real_space_refine model.pdb map.mtz ncs.constraints.pdbout
```

9. Use NCS to generate the ncs operators and ncs constraints automatically (default):

```
phenix.real_space_refine model.pdb map.mtz ncs.constraints=on pdbout
```

NCS groups are defined in the output file "real_space_refine_PDB.ncs_spec" and can be edited and used in subsequent runs:

```
phenix.real_space_refine model.pdb map.mtz
ncs.constraints.ncs_group_1.ncs_spec=real_space_refine_PDB.ncs_spec
```

10. Use NCS operators and NCS constraints explicitly:

```
phenix.real_space_refine model.pdb map.mtz
ncs.constraints.ncs_group_1.ncs_spec=ncs.ncs_spec
```

IMPORTANT: records are parsed in PDB file they will be used to construct rotamers. Rotamers are fitted into the map and then regularized. Ncs constraints are applied to rotamers from the most recent, rotamer-fitted, specific residues (or the specified residues). Not all residues fit well into density, some of rotamer fitted residues is almost meaningless and will be regularized away. Ncs constraints are applied to the regularized rotamers. Ncs constraints are not applied to the rest of the model.

Bfac: Ncs constraints are not applied to bfactors (only to the coordinates and rotamers given a model with ncs constraints):

```
phenix.secondary_structure.inputs model.pdb format=pdb
```

and the pdb output is produced. Use that pdbfile for restraints, ready to use for refinement:

```
phenix.real_space_refine model.pdb map.mtz type.pdb
```

Note NS annotation programs (ss detection) for CIFs results in all seven (6) consecutive prolines being annotated as helix, which is not good. Use PDB format instead. Note that ss annotation is not used by default, only if ss.restraints.enabled=True. Reason for this is because it is better to use that provided NS annotation (as all cis-prolines in it is taken into account) than to make it from scratch (which is default).

11. Rotamer fitting is performed automatically if model is scored as poor and then verify if it improves the fit to the map. Rotamer fitting is not applied to residues with CB deviations.

12. Metals between sites and metals in determined automatically to achieve specified ion coordination geometry (default: octahedral for TM and tetrahedral for others). Use the following: phenix.ion.identify -h for more details. Use the output of the identify manually:

```
phenix.real_space_refine model.pdb map.mtz ion.pdb
```

13. Number of refinement macro-cycles defaults to 5, which is sufficient in most cases. If model needs more cycles to converge, use `macro_cycles=` to specify a different number of cycles:

```
phenix.real_space_refine model.pdb map.mtz macro_cycles=10
```

14. It is possible to define a bond between any pair of atoms, any number of bonds, chiralities, or planarities using the "Phenix Geometry Restraints Manager" (PGRM) syntax. Bonds, chiralities, planarities, torsions, chirsums, planrms and planbonds restraints are supported. The example below defines a bond between atoms with serial numbers 1 and 2 with ideal distance of 1.54 and sigma of 0.02:

```
bond
atom_selection1 = "serial 1"
atom_selection2 = "serial 2"
distance_ideal = 1.54
sigma = 0.02
```

Note that user-supplied NCS groups will be filtered at all times. More on the Note

NCS groups definitions can be obtained using SSM or combined from two:

```
phenix.ncs_search model.pdb
```

NCS operators are defined if NCS constraints are used. To disable refinement of NCS operators use `ncs.operators.refinement=false`:

```
phenix.real_space_refine model.pdb map.mtz
ncs.constraints=true ncs.operators.refinement=false
```

15. Refinement of NCS operators is controlled by `ncs.operators.refinement` keyword:

```
phenix.real_space_refine model.pdb map.mtz
ncs.constraints=true ncs.operators.refinement=true
```

IMPORTANT: records are parsed in PDB file they will be used to construct rotamers. Rotamers are fitted into the map and then regularized. Ncs constraints are applied to rotamers from the most recent, rotamer-fitted, specific residues (or the specified residues). Not all residues fit well into density, some of rotamer fitted residues is almost meaningless and will be regularized away. Ncs constraints are applied to the regularized rotamers. Ncs constraints are not applied to the rest of the model.

Bfac: Ncs constraints are not applied to bfactors (only to the coordinates and rotamers given a model with ncs constraints):

```
phenix.secondary_structure.inputs model.pdb format=pdb
```

and the pdb output is produced. Use that pdbfile for restraints, ready to use for refinement:

```
phenix.real_space_refine model.pdb map.mtz type.pdb
```

Note NS annotation programs (ss detection) for CIFs results in all seven (6) consecutive prolines being annotated as helix, which is not good. Use PDB format instead. Note that ss annotation is not used by default, only if ss.restraints.enabled=True. Reason for this is because it is better to use that provided NS annotation (as all cis-prolines in it is taken into account) than to make it from scratch (which is default).

16. Refinement of NCS operators is controlled by `ncs.operators.refinement` keyword:

```
phenix.real_space_refine model.pdb map.mtz
ncs.constraints=true ncs.operators.refinement=true
```

17. Number of refinement macro-cycles defaults to 5, which is sufficient in most cases. If model needs more cycles to converge, use `macro_cycles=` to specify a different number of cycles:

```
phenix.real_space_refine model.pdb map.mtz macro_cycles=10
```

18. It is possible to define a bond between any pair of atoms, any number of bonds, chiralities, or planarities using the "Phenix Geometry Restraints Manager" (PGRM) syntax. Bonds, chiralities, planarities, torsions, chirsums, planrms and planbonds restraints are supported. The example below defines a bond between atoms with serial numbers 1 and 2 with ideal distance of 1.54 and sigma of 0.02:

```
bond
atom_selection1 = "serial 1"
atom_selection2 = "serial 2"
distance_ideal = 1.54
sigma = 0.02
```

Note that user-supplied NCS groups will be filtered at all times. More on the Note

NCS groups definitions can be obtained using SSM or combined from two:

```
phenix.ncs_search model.pdb
```

NCS operators are refined if NCS constraints are used. To disable refinement of NCS operators use `ncs.operators.refinement=false`:

```
phenix.real_space_refine model.pdb map.mtz
ncs.constraints=true ncs.operators.refinement=false
```

19. Refinement of NCS operators is controlled by `ncs.operators.refinement` keyword:

```
phenix.real_space_refine model.pdb map.mtz
ncs.constraints=true ncs.operators.refinement=true
```

Inputs

Outputs

Keywords and parameters

```
{
  "mesh_specification": {
    "element_specification": {
      "fluid": {
        "element": "fluid",
        "polynomial_degree": 4,
        "quadrature_points": 5,
        "mass_matrix_diagonalization": true,
        "gamma": 1.4,
        "riemann_solver": "HLLC",
        "boundary_conditions": {
          "periodic": true,
          "inflow": {
            "density": 1.0,
            "velocity": [1.0, 0.0, 0.0],
            "pressure": 1.0
          },
          "outflow": {
            "pressure": 1.0
          },
          "wall": {
            "velocity": [0.0, 0.0, 0.0],
            "thermal": "adiabatic"
          }
        }
      }
    }
    "boundary_specification": {
      "boundary_condition_mapping": {
        "x_min": "inflow",
        "x_max": "outflow",
        "y_min": "wall",
        "y_max": "wall",
        "z_min": "periodic",
        "z_max": "periodic"
      }
    }
    "mesh_topology": {
      "type": "hexahedral",
      "cubed_sphere": false,
      "periodicity": [false, false, false]
    }
    "coordinate_transformation": {
      "type": "identity",
      "parameters": {}
    }
    "mesh_quality_checks": {
      "jacobian_positivity": true,
      "max_aspect_ratio": 10.0,
      "min_element_volume": 1.e-12
    }
    "mesh_partitioning": {
      "method": "metis",
      "number_of_partitions": 128,
      "ghost_layer_width": 1
    }
    "mesh_output": {
      "format": "hdf5",
      "write_partition_info": true,
      "write_boundary_info": true,
      "write_quality_metrics": true
    }
  }
  "initial_condition": {
    "type": "analytic",
    "expression": {
      "density": "1.0 + 0.2*sin(2*pi*(x+y+z))",
      "velocity_x": "1.0",
      "velocity_y": "0.0",
      "velocity_z": "0.0",
      "pressure": "1.0"
    }
    "checkpoint": false
    "checkpoint_file": null
    "checkpoint_time": null
    "checkpoint_format": null
    "checkpoint_compression": null
    "checkpoint_verify_checksum": null
    "checkpoint_write_ghost": null
    "checkpoint_write_metadata": null
    "checkpoint_overwrite": null
    "checkpoint_interval": null
    "checkpoint_keep_last": null
    "checkpoint_directory": null
    "checkpoint_prefix": null
    "checkpoint_time_tolerance": null
    "checkpoint_step_tolerance": null
    "checkpoint_restart_mode": null
    "checkpoint_restart_file": null
    "checkpoint_restart_time": null
    "checkpoint_restart_step": null
    "checkpoint_restart_verify": null
    "checkpoint_restart_fallback": null
    "checkpoint_restart_ignore_mismatch": null
    "checkpoint_restart_ignore_missing": null
    "checkpoint_restart_ignore_extra": null
    "checkpoint_restart_ignore_corrupt": null
    "checkpoint_restart_ignore_incompatible": null
    "checkpoint_restart_ignore_all": null
    "checkpoint_restart_ignore_none": null
    "checkpoint_restart_ignore_partial": null
    "checkpoint_restart_ignore_stale": null
    "checkpoint_restart_ignore_unknown": null
    "checkpoint_restart_ignore_version": null
    "checkpoint_restart_ignore_checksum": null
    "checkpoint_restart_ignore_header": null
    "checkpoint_restart_ignore_footer": null
    "checkpoint_restart_ignore_metadata": null
    "checkpoint_restart_ignore_data": null
    "checkpoint_restart_ignore_mesh": null
    "checkpoint_restart_ignore_boundary": null
    "checkpoint_restart_ignore_initial": null
    "checkpoint_restart_ignore_time": null
    "checkpoint_restart_ignore_step
```

rebuild_model

Phenix (Python-based Hierarchical Environment for Integrated Xtallography)

Model rebuilding keeping connectivity and allowing insertions and deletions

Author(s):

- Ralf Grosse-Kunstleve, Tom Terwilliger

Purpose

Rebuild a model, keeping all connectivity the same but allowing insertions and deletions.

How rebuild_model works:

Rebuild a model, keeping all connectivity the same but allowing insertions and deletions.

Rebuilding is done using a chain of one-residue-at-a-time substitutions in segments of about 10-20 residues and keeping the connectivity of the chain and the connectivity of the ends.

Each segment is rebuilt with several different base rotamers (default base rotamers are refinement), fixing connectivity and using the best fit to the electron density.

For each base rotamer, a sequence of substitutions alpha is carried out (typically refinement, the base rotamer replacement of one residue, regeneration, and another replacement of one residue).

The best sequence of substitutions is then selected and the segment is rebuilt.

If there are multiple chains in your model, each is rebuilt separately.

If there are multiple chains in your model, the connectivity of the ends of refinement cycle is 1 (otherwise there are 2 normal ends and also all of the substitutions alpha except the base rotamer

Examples

Standard run of rebuild_model:

Running rebuild_model is easy. Put the command line you can type

phenix.rebuild_model model.pdb map.ccp4 resolution=3.0 seq_file=seq.dat

This will rebuild the model.pdb based on the map.ccp4 map and at a resolution of 3.0 using the sequence.

Possible Problems

Specific limitations and problems:

Literature

Additional information:

List of all available keywords

```
seq_file: None                      ~> TYPE: 1-WORD-LEN, not used on command line

input_file:
  pdb_file: None
  map_file: None
  phasefile: None
  mtz_label:
    fobs_label: None
    hl_label: None
    free_label: None
    phase_label: None

output:
  model_file: None                  ~> Output file name
  log: None                         ~> Redirect file name
  overwrite: True                   ~> If specified, can overwrite output files (default)
  mtz_label:
    fobs_label: FOBS                ~> Input fobs label
    hl_label: HL                    ~> Input HL label
    free_label: FREE                ~> Input free label
    phase_label: PHIB               ~> Output phase label

output:
  model_file: None                  ~> Output file name
  log: None                         ~> Redirect file name

rebuild_model:
  substitution_definition: True     ~> Use substitution definitions
  refine_alpha: None                ~> Refinement alpha (use alpha to find refined) default is 1 for refinement and 0 for rotamers
  delta_cutoff: 1.5                 ~> Cutoff for delta to be allowed in fit (1.5)
  base_alpha: None                  ~> Base alpha (0 for rotamers)
  base_rotamers: 1                  ~> Number of base rotamers to try (default is 1 for refinement)
  base_substitution_set_of_models:  ~> Substitution sequence set to apply (all if omitted) default
    None
  segment_length: None              ~> Length of segment to rebuild (about this size)

  rotamer_name:
    rotamer_name: ANY               ~> Rotamer restriction of any
    residue_rotamers: 1-3           ~> 1=backbone,2=beta,3=gamma rotamers (or
    substituting_model: 1-positive  ~> Substitution model(s) to use (1=first substitution,
                                       2=second substitution, 3=third substitution, 4=fourth
                                       substitution, 5=fifth substitution, 6=sixth substitution
                                       (default is 1)
    alpha_mtz: None                 ~> Alpha mtz file (output from refinement)
    segment: None                   ~> Segment of alpha(s) to apply (all if omitted)

  alpha:
    alpha: 1.0                      ~> Number of alpha(s) to apply (all if omitted)
    alpha_number_to_substitute: 1-positive ~> Alpha(s) to apply for substitution (default is 1)
                                       (1=first alpha, 2=second alpha, 3=third alpha, 4=fourth alpha,
                                       5=fifth alpha, 6=sixth alpha)
    weight: None                    ~> Alpha weight (apply this weight to the alpha value
                                       before substituting into the model)
    segment: None                   ~> Segment

  model:
    model: 1                        ~> Number of alpha(s) to apply (all if omitted)
    model_number_to_substitute: 1-positive ~> Model(s) to apply substitution (default is 1)
                                       (1=first model, 2=second model, 3=third model, 4=fourth model,
                                       5=fifth model, 6=sixth model)
    weight: None                    ~> Model weight (apply this weight to the model before
                                       substituting into the model)
    segment: None                   ~> Segment

  segment:
    segment: 1                      ~> Segment of alpha(s) to apply (all if omitted)
    model_number_to_substitute: 1-positive ~> Model(s) to apply substitution (default is 1)
                                       (1=first model, 2=second model, 3=third model, 4=fourth model,
                                       5=fifth model, 6=sixth model)
    weight: None                    ~> Segment weight (apply this weight to the segment before
                                       substituting into the model)
    segment: None                   ~> Segment

  write_intermediate_files: True    ~> Write intermediate files
  output_dir: None                  ~> PDB/mtz/ccp4 output required for output directory
```

mvlpneu8_spun_artsrb

Phenix *Multi-level Hierarchical Mechanism for Integrated Multigrids*

Spun material, sheet, artsrb: composite serrous wrap (such as Kuat, Tinsel, Phenix, Rock, and Arm)

Inputs:

- the sark reflectivity data (files in Ionic R-Tree flags, and optionally RL coefficients. It can be in level representation or in compressed representation
- physical spacing which defines the grid. Should be used in case there are multiple chrome in different spacing which defines the grid
- Model file (PDB or ArcCET) with input bonds

Intermediate Arrays:

- atoms-material, sheet, artsrb model with BAN-RC (ids, label "CORE"
- atoms-material, sheet, artsrb model with BAN-RC (ids, label "SHELL"

Output:

- All the sark data arrays. Depending on the input data, the following arrays may be present:
  - FIXED - data from input reflectivity file
  - SUPERB - corresponding flagrate
  - ALL_ATOMS - all atoms in the sark (i.e. bact)
  - ALL_ATOMS_SUPERB - corresponding flagrate. See phenix.hierarchical for details
  - MASKED - corresponding phenix
  - FIXED_SUPERB - corresponding flagrate
  - PHIFCALC - corresponding phenix
  - PHIFCALC_SUPERB - corresponding flagrate. See phenix.hierarchical for details
  - MASKED - corresponding phenix
  - MASKED_SUPERB - corresponding flagrate. See phenix.hierarchical for details
  - PHIFCALC - corresponding phenix
  - PHIFCALC_SUPERB - corresponding flagrate
  - SCAT - RL coefficients used in sark calculation for DVA-SAFL flags
  - SCAT_SUPERB - corresponding flagrate. See phenix.hierarchical for details
  - FULL - RL coefficients from input reflection file
  - FULL_SUPERB - corresponding flagrate. See phenix.hierarchical for details
  - FULL - RL coefficients from input reflection file
  - FULL_SUPERB - corresponding flagrate. See phenix.hierarchical for details
  - RLCoeff0 - RL coefficients from the model [C1-N-CA]
  - RLCoeff1 - RL coefficients from the model [C1-N-CD]
  - RLCoeff2 - RL coefficients from the model [C1-N-H]
  - RLCoeff3 - RL coefficients from the model [C1-N-O]
  - RLCoeff4 - RL coefficients from the model [C1-N-OT]
  - RLCoeff5 - RL coefficients from the model [C1-N-OT]
  - RLCoeff6 - RL coefficients from the model [C1-N-OT]
  - RLCoeff7 - RL coefficients from the model [C1-N-OT]
  -

end

Python based Hierarchical Mechanism for Enzymes Bioligands

Restraints Editor Especially Ligands (REEL)

Contents:

- Author
- Scope
- Dictionaries
- Special Treatment
- Output
- Usage
- Manual
- Tutorial
- Applications

Author

Ingo W. Morsky

Parameters

The parameters concerns of a ligand using a Graphical User Interface (GUI) including a 3D view of the ligand and a table view of the topology.

Screen Shots

Placing CA atoms in a map with refine_ca_model

Author(s):

- refine_ca_model Tom Terwilliger

Purpose

The tool refine_ca_model is a tool for adjusting CA/P/K positions in a preliminary model to increase its consistency with a density map and chain tracing.

Usage

How refine_ca_model works:

The refine_ca_model tool takes a set of CA positions, and optionally, a set of CB positions. It adjusts the CA/P/K positions to increase their consistency with a density map and with chain tracing. It also adjusts the CB positions so that they are close to the CA/P/K distance as close to 1.9 Å as possible.

Using refine_ca_model:

The tool refine_ca_model is usually run automatically as part of trace_and_build. However you can run it independently if you have a CA/P/K model and a map.

Input map file: The map file should cover the model as needed.

Resolution: Specify the resolution of your map (usually the resolution defined by your half-dataset Fourier shell correlation).

CA/P/K model: Supply a model that at least has CA positions. If you supply CB positions the new CB positions will be adjusted to be close to 1.9 Å.

Examples

Standard use of refine_ca_model:

You can use refine_ca_model to adjust a CA/P/K model based on a cryo-EM map:

```
phenix.refine_ca_model map.mrc resolution=3.4 ca_in.pdb
```

Possible Problems

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
phenix.refine_ca_model
  ca_in.pdb "" None                  ca_in.pdb PDBREF.SEQ, set_ext or command line
  map_in.ccp4 "" None
  seq_in.seq "" None                 file with SEQRES data. May have origin in ala location.
  cb_in.pdb "" None                  Input PDB file with CB positions to be adjusted (keep atoms ignored
  output_dir
    output_prefix_format = None_str  Output prefix format (if specified). Inserts one Rmsd (1/1.5) and
                                     one Rmsd (1/1.5) and one cycle number (if more than one cycle)
                                     Rmsd and cycle number are inserted in place of %1f and %d
                                     Rmsd and cycle number are also inserted into output dir name
    seq_dir = None                   Sequence directory
  output_files
    pdb_out = None                   Pdb/mtz/ccp4 file for pdb output.
    nonbonding_dmin = 2.5            Minimum nonbonding distance for nonbonding factor calculation.
                                     Nonbonding factor is 1 if nonbonding distance is larger than this.
    chain_length = 4000000           Chain length for MAXIMUM
    cb_distance = 1.9 A              Ideal distance between CA and CB
    output_cycles = None             Write output at the end of this or these cycles (1 is first)
                                     Default is only at the end. Output is in current directory
                                     Output cycle 0 is the starting model. Output cycle -1 is the last
                                     Output cycle -2 is the next-to-last cycle, etc. Output cycle 999
                                     includes all output files from all cycles
    output_cycles_interval = 1       Interval of output files to write
    write_all_cycles = False         Write out all cycles (default is only the last one)
    cb_radius_for_ca = 4.25          Radius around CA for consideration of CB when the nonbonding
                                     distance with CB is not the same as the nonbonding distance for
                                     another atom and the CB is closer than 1.9 to the CA
    cb_scale = 0.95                  Scale factor for CB distance (1.9 times this factor)
    ptmp_cut = None                  Write intermediate maps/models, cut-from-site based on map
  refine
    refine_ptmp_length = 10          Length of segments to refine
    refine_ptmp_frac = None          Refine ptmp_frac of all sites
    refine_ca = True                 Refine CA positions
    refine_cb = True                 Cbeta refined to refine
    refine_ca_with_cb = False        CA refined with Cbeta if refined
    refined_ca = None                CA refined positions if refined
    new_interatom = 3.8              Interatom ca interpoint
  weight
    weight_cb_ca_dist = 1.0          Weight on CB-CA distance
    weight_ca = 1                    Weight on CA initial positions
    weight_nonbonding_factor = 1     Weight on nonbonding
    weight_density = 1.0             Weight on density on map (0 ignore)
    weight_cb_density = 1.0          Weight on density on cb atoms, between CA atoms, and CB positions
  other
    nproc = 1                        Number of processors to use
    verbose_level = VERYVEB          Verbose level
    output_log = None                Output log file
    save_loading_coefficients = False Save the coefficients representing different form assessments
                                     Coefficients are saved in a file named PREF.coef where PREF is the
                                     output log file (default)
    verbose = True
    skip_optimization = False        Skip optimization
    write_log_only = False           Write only output log (not coordinates, coefficients, or maps) and
                                     exit
  dir
    output_dir = None                DEF-specify parameter required for output directory
```

The phenix.refine graphical interface

Contents

- GUI overview
- Video tutorial
- Configuration
- Run phenix.refine
- Quick Help
  - Quick Help (phenix.refine's reference manual)
  - Tooltips and hyperlinks
- Identifying and editing TLS groups
- Analysis automation
- Run phenix.refine
- Manual options
- Automatically generating TLS groups
- Other options
- After refinement
- Frequently Asked Questions
- Acknowledgements
- References

GUI overview

The graphical interface for phenix.refine runs the unmodified command line version. Default settings are provided for most options, and only those options which are required for a particular run are displayed. Advanced options are handled in a non-obvious way, this document describes the behavior of the GUI only. See phenix.refine documentation and tutorials for more information on phenix.refine. There is also a Frequently Asked Questions about phenix.refine.

At present the GUI has the following capabilities in addition to the features included in phenix.refine:

- Automatically generate phenix.refine input files from PDB/mtz files
- Selection of reference models and generation of restraints files
- Automatically generate TLS groups using phenix.tls_analysis
- Assign specific defined settings and options
- Run phenix.refine with default options
- Run phenix.refine with modified options and monitoring refinement
- Run phenix.refine with automatically generated TLS groups
- Automatic comparison of structure quality measures
- Other miscellaneous features

Video Tutorial

The tutorial video is available on the Phenix YouTube channel and covers the following topics:

- Basic run
- Generating phenix.refine input files
- Analysis of phenix.refine default parameters using the data from this tutorial

Configuration

The GUI will attempt to guess the purpose of PDB and mtz files, but you may change this by right-clicking on the file and selecting the appropriate option. Files may also be added or removed using the buttons on the left and their settings modified using the drop-down menu.

Once the input files are selected, the GUI will attempt to determine the appropriate command-line options. Most parameters will be defaulted automatically. Appropriate cancel dialog for reflection files and any dialog for the ligand restraints will be displayed if needed. Once the input files are selected, the GUI will display the main phenix.refine control panel. The Phenix Help button provides access to phenix.refine documentation and tutorials. The Run button will start the refinement. The Stop button will terminate the refinement. The Quit button will terminate the GUI and shutdown the server.

Refinement settings

The main refinement settings are displayed in the refinement window. Most of these controls will open additional dialogs or displays or modify some aspect of the calculation. In many cases, you can open these windows or dialogs before or after the calculation is started. Some options will be disabled until the calculation is started, and some options may disappear when they are no longer relevant. Most of the options are described in the Quick Help dialog.

Most of the refinement options presented on this tab essentially full mirror their categories.

- **Model parameterization**: The determinant which properties of the model will be refined and which will be held fixed. Options include refinement of individual atomic coordinates, individual atomic B-factors, occupancies, or rigid body groups (groups of rigid atoms) and TLS groups (groups of atoms with common motion). Refinement of individual atomic coordinates and individual atomic B-factors is the default. Refinement of rigid body groups requires a separate file defining the groups. Refinement of TLS groups requires a separate file defining the groups.
- **Optimization target**: The definition the function to be minimized. By default this is a target the combines the model-data agreement with a geometry restraints term. Other options include a pure model-data agreement target, a pure geometry restraints target, a model-data agreement target with a Bayesian bias, and a model-data agreement target with a Bayesian bias and a geometry restraints term.
- **Optimization method**: The standard optimization method used in phenix.refine and xtalmin. Options include conjugate gradient minimization, LBFGS minimization, and simulated annealing. Simulated annealing offers a significantly wider region of convergence, but at the cost of increased runtime.

The default options have been chosen to work well for typical refinement scenarios at moderate resolutions, which are defined as 2.0 Å and lower for X-ray data and 3.0 Å and lower for neutron data. Higher resolution data may be treated as if it is low resolution if the ratio of observations to number of refined parameters is too low.

Parameterization (refinement strategy)

The refinement strategy can be further modified by manipulating various refinement targets, including weights and additional restraints.

- **Target function**: Describes the calculation of model-data fit to experimental data. For X-ray data, the default is maximum likelihood (ML) for all but very low resolution data, where least squares (LS) is used. For neutron data, ML is not suitable for general use. The least squares (LS) target is only valid for data with a Gaussian error distribution, which is not true for neutron data. The default for neutron data is a modified least squares target that includes a Bayesian bias to the model-data agreement. Other options include a pure model-data agreement target, a model-data agreement target with a Bayesian bias, and a model-data agreement target with a Bayesian bias and a geometry restraints term.
- **Weight**: Controls the weight of the model-data agreement target relative to the geometry restraints target. The default is to use a weight of 1.0 for X-ray data and 0.5 for neutron data. Other options include a fixed weight, a weight that varies with resolution, and a weight that varies with the number of observations. A fixed weight of 1.0 is recommended for most X-ray data, and a fixed weight of 0.5 is recommended for most neutron data.
- **Individual B-factors**: Controls the refinement of individual atomic B-factors. Options include refinement of individual B-factors, individual B-factors with a restraint to a fixed value, and individual B-factors with a restraint to a fixed value with a variable weight. The default is to refine individual B-factors with a restraint to a fixed value of 20 Å^2. Refinement of individual B-factors is recommended for most data at resolutions 3.0 Å and better, and a restraint to a fixed value is recommended for most data at resolutions 3.0 Å and worse.
- **Occupancies**: Controls the refinement of occupancies. Options include refinement of occupancies, refinement of occupancies with a restraint to a fixed value, and refinement of occupancies with a restraint to a fixed value with a variable weight. The default is to refine occupancies with a restraint to a fixed value of 1.0. Refinement of occupancies is recommended for most data at resolutions 3.0 Å and better, and a restraint to a fixed value is recommended for most data at resolutions 3.0 Å and worse.
- **Hydrogens**: Controls the refinement of hydrogens. Options include refinement of hydrogens, refinement of hydrogens with a restraint to a fixed value, and refinement of hydrogens with a restraint to a fixed value with a variable weight. The default is to refine hydrogens with a restraint to a fixed value of 1.0. Refinement of hydrogens is recommended for most data at resolutions 2.0 Å and better, and a restraint to a fixed value is recommended for most data at resolutions 2.0 Å and worse.
- **Automatic weight**: Controls the automatic weight optimization. Options include automatic weight optimization, automatic weight optimization with a variable weight, and no automatic weight optimization. The default is to use automatic weight optimization with a variable weight. Automatic weight optimization is recommended for most data at resolutions 3.0 Å and better.
- **Secondary structure restraints**: Controls the application of secondary structure restraints. Options include no secondary structure restraints, secondary structure restraints, and secondary structure restraints with a variable weight. The default is to use secondary structure restraints with a variable weight. Secondary structure restraints are recommended for most data at resolutions 3.0 Å and better.
- **Ramachandran restraints**: Controls the application of Ramachandran restraints. Options include no Ramachandran restraints, Ramachandran restraints, and Ramachandran restraints with a variable weight. The default is to use Ramachandran restraints with a variable weight. Ramachandran restraints are recommended for most data at resolutions 3.0 Å and better.
- **Rotamer restraints**: Controls the application of rotamer restraints. Options include no rotamer restraints, rotamer restraints, and rotamer restraints with a variable weight. The default is to use rotamer restraints with a variable weight. Rotamer restraints are recommended for most data at resolutions 3.0 Å and better.
- **Reference model restraints**: Controls the application of reference model restraints. Options include no reference model restraints, reference model restraints, and reference model restraints with a variable weight. The default is to use reference model restraints with a variable weight. Reference model restraints are recommended for most data at resolutions 3.0 Å and better.
- **Reference model selection**: Controls the selection of reference model restraints. Options include all reference model restraints, reference model restraints for backbone atoms, and reference model restraints for C-alpha atoms. The default is to use reference model restraints for all atoms. Reference model restraints for backbone atoms are recommended for most data at resolutions 3.0 Å and better.

Optimization methods and other options

Several other options are available for the types of optimization used. These typically apply directly, except as noted.

- **Automatically optimize/refine/run n times**: Controls the number of times the refinement is run. Generally, automatically optimize (automatically) unless approximate. This usually only affects the number of times the refinement is run, but some options may be affected by this setting.
- **Optimize/refine/run n times**: Controls the number of times the refinement is run. Generally, optimize/refine/run n times (n) unless approximate. This usually only affects the number of times the refinement is run, but some options may be affected by this setting. Generally, the number of times the refinement is run is the number of times the refinement is run, but some options may be affected by this setting. For example, the number of times the refinement is run may be affected by the number of times the refinement is run, but some options may be affected by this setting.
- **Approximate**: Controls the approximation of the refinement. Generally, approximate (approximate) unless approximate. This usually only affects the number of times the refinement is run, but some options may be affected by this setting.
- **Optimize solvent**: Automatically adds and removes solvent atoms as necessary. This is usually recommended for most data at resolutions 3.0 Å and better, and is required for most data at resolutions 2.0 Å and better.
- **Fast refinement**: Controls solvent picking to fast mode (default) or slow mode. Fast mode is usually sufficient for most data at resolutions 3.0 Å and better, and slow mode is required for most data at resolutions 2.0 Å and better.
- **Optimize solvent**: Automatically adds and removes solvent atoms as necessary. This is usually recommended for most data at resolutions 3.0 Å and better, and

```
phenix.refine model.pdb data.mtz ncs=auto
```

This will automatically detect 2-fold NCS in the data.

Refinement of group occupancy for ligands in phenix.refine does not change the original distribution of its occupancy. Instead, it adds a new occupancy group for the ligand and refines it. This is done because it is not clear how to refine occupancy of a group if it is spread across several NCS copies. Refinement of group occupancy is supported for ligands only.

Atoms with occupancies lower than 0.01 are ignored by phenix.refine, and the rest are kept as is. Atoms with occupancies lower than 0.01 are also ignored by most other PHENIX programs.

- Refinement of individual ADP (isotropic, anisotropic)

By default phenix.refine refines isotropic atom ADP, and the rest remains as is. Refinement of individual ADP is supported for isotropic and anisotropic ADP. Refinement of individual ADP is supported for all atoms.

- Refinement of individual isotropic ADP for a mixed protein/ligand structure

If NCS is present, phenix.refine automatically applies NCS restraints to ADP. Refinement of individual ADP is supported for all atoms.

- Refinement of individual ADP (isotropic, anisotropic)

```
phenix.refine model.pdb data.mtz adp=individual
```

By default, phenix.refine refines isotropic atom ADP, and the rest remains as is. Refinement of individual ADP is supported for isotropic and anisotropic ADP.

- Refinement of individual isotropic ADP for a mixed protein/ligand structure

```
phenix.refine model.pdb data.mtz adp=individual
```

If NCS is present, phenix.refine automatically applies NCS restraints to ADP. Refinement of individual ADP is supported for all atoms.

- Refinement of individual isotropic ADP for a mixed protein/ligand structure in cases when NCS is present

```
phenix.refine model.pdb data.mtz adp=individual
```

If NCS is present, phenix.refine automatically applies NCS restraints to ADP. Refinement of individual ADP is supported for all atoms.

- Refinement of individual isotropic ADP for a mixed protein/ligand structure in cases when NCS is present and it is desired to turn off NCS restraints

refinement_file_editor

Refinement at high resolution (higher than approx. 1.0 Angstrom)

Guidelines for refinement at high resolution (higher than approx. 1.0 Angstrom):

- Use the most recent available Phenix version. If the phenix.refine GUI wizard is used then:
  - phenix.refine dev-4481 or dev-4482
  - By default phenix.refine will refine occupancies of all sites as they model no alone with exactly 1.00 occupancy. This is not good at high resolution. Use occupancy.refinement.remove=True option to remove sites with occupancy less than 0.1 (default is 0.01) and then refine occupancies. Use occupancy.refinement.refine=occupancies to refine occupancies. Use occupancy.refinement.refine=occupancies+adp to refine both occupancies and ADP. Use occupancy.refinement.refine=occupancies+adp+sites to refine occupancies, ADP and coordinates. Use occupancy.refinement.refine=occupancies+sites to refine occupancies and coordinates. Occupancies should be used for refinement of TLS occupancies. occupancies.refine=occupancies
- Use phenix.ordered_solvent to add ordered solvent molecules. Use ordered_solvent.mode=2mfo-dfc with high 2mFo-DFc sigma cutoff (default is 1.0) to remove ordered solvent molecules. Use ordered_solvent.mode=mfo with high MFo-DFc sigma cutoff (default is 3.0) to remove ordered solvent molecules. Use ordered_solvent.mode=mfo+2mfo-dfc to remove ordered solvent molecules by both criteria.
- It is a good idea to manually remove ordered solvent molecules that are not supported by the data. Use phenix.refine ordered_solvent.mode=2mfo-dfc ordered_solvent.mask_out=True to make sure that the newly added solvent sites are meaningful. Use ordered_solvent.mask_out=True to make sure that the solvent sites do not clash with other atoms. Use ordered_solvent.mask_out=False to keep all solvent sites.
- Use phenix.ordered_solvent -d -m 2mfo-dfc -s 1.0 -o -r -c -p -n -v -w -t 0.5 -f -a -b -l -i -x -y -z -e -h -k -u -j -q -g -m -d -s -o -r -c -p -n -v -w -t

Phenix *Action-based Macromolecular Refinement for Integrated Crystallography*

reflection file tools

phenix.reflection_file_converter

Purpose:

phenix.reflection_file_converter is a simple utility program that allows a straightforward conversion of many reflection file formats into one, as long as it is supported in cctbx/Boost. Currently, conversion between datasets and a single output file is not supported.

Keywords:

Topics:

```
phenix.reflection_file_converter --help
```

Usage:

```
usage: phenix.reflection_file_converter [options] reflection_file ...

  Options:
    --version  show program's version number and exit
    -h, --help, -?, -H, -Help, --Help, --help=hidden, --help=all, --help=noalias, --help=expert, --help=hidden,
                --help=all, --help=noalias, --help=expert, --help=hidden, --help=all, --help=noalias, --help=expert,
                --help=hidden, --help=all, --help=noalias, --help=expert, --help=hidden, --help=all, --help=noalias,
                --help=expert, --help=hidden, --help=all, --help=noalias, --help=expert, --help=hidden, --help=all,
                --help=noalias, --help=expert
```

Reflection Statistics

phantis_reflection_statistics

Comparisons between multiple datasets are available via the `phantis_reflection_statistics` command:

```
Usage: phantis_reflection_statistics [options] reflection_file [...]

Options:
  -h, --help            Show this help message and exit
  -v, --version         Show program's version number and exit
  -c, --cancel-on-error=CANCEL_ON_ERROR
                        Cancel if any error occurs
  -q, --quiet=QUIET     Quiet (no output)
  -f, --force=FORCE     Force (ignore warnings)
  -n, --no-header=NO_HEADER
                        Do not output header (for quiet) Used
                        with -q/--quiet
  -o, --output=OUTPUT   Write output to file instead of stdout
  -d, --delimiter=DELIMITER
                        Delimiter (default: ',')
  -r, --recursive=RECURSIVE
                        Recursive (scan folders) Default:
                        False
  -t, --time-limiting=TIME_LIMIT
                        Time limit for the run
  -p, --parallel=PARALLEL
                        Number of all the cores aspects of
                        connection
  -i, --print-indentation=PRINT_INDENT
                        Indentation for the output JSON in the
                        pretty-printed mode
```

Example: `phantis_reflection_statistics 3D3D.dat 3D3D.dat 3D3D.dat`

`phantis_reflection_statistics` calculates the following statistics: MFD, Skewness, CV%, SHELXC, for each of the datasets found in the reflection file the output shows a line like the following:

```
3D3D.dat,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48,49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96,97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144,145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,180,181,182,183,184,185,186,187,188,189,190,191,192,193,194,195,196,197,198,199,200,201,202,203,204,205,206,207,208,209,210,211,212,213,214,215,216,217,218,219,220,221,222,223,224,225,226,227,228,229,230,231,232,233,234,235,236,237,238,239,240,241,242,243,244,245,246,247,248,249,250,251,252,253,254,255,256,257,258,259,260,261,262,263,264,265,266,267,268,269,270,271,272,273,274,275,276,277,278,279,280,281,282,283,284,285,286,287,288,289,290,291,292,293,294,295,296,297,298,299,300,301,302,303,304,305,306,307,308,309,310,311,312,313,314,315,316,317,318,319,320,321,322,323,324,325,326,327,328,329,330,331,332,333,334,335,336,337,338,339,340,341,342,343,344,345,346,347,348,349,350,351,352,353,354,355,356,357,358,359,360,361,362,363,364,365,366,367,368,369,370,371,372,373,374,375,376,377,378,379,380,381,382,383,384,385,386,387,388,389,390,391,392,393,394,395,396,397,398,399,400,401,402,403,404,405,406,407,408,409,410,411,412,413,414,415,416,417,418,419,420,421,422,423,424,425,426,427,428,429,430,431,432,433,434,435,436,437,438,439,440,441,442,443,444,445,446,447,448,449,450,451,452,453,454,455,456,457,458,459,460,461,462,463,464,465,466,467,468,469,470,471,472,473,474,475,476,477,478,479,480,481,482,483,484,485,486,487,488,489,490,491,492,493,494,495,496,497,498,499,500,501,502,503,504,505,506,507,508,509,510,511,512,513,514,515,516,517,518,519,520,521,522,523,524,525,526,527,528,529,530,531,532,533,534,535,536,537,538,539,540,541,542,543,544,545,546,547,548,549,550,551,552,553,554,555,556,557,558,559,560,561,562,563,564,565,566,567,568,569,570,571,572,573,574,575,576,577,578,579,580,581,582,583,584,585,586,587,588,589,590,591,592,593,594,595,596,597,598,599,600,601,602,603,604,605,606,607,608,609,610,611,612,613,614,615,616,617,618,619,620,621,622,623,624,625,626,627,628,629,630,631,632,633,634,635,636,637,638,639,640,641,642,643,644,645,646,647,648,649,650,651,652,653,654,655,656,657,658,659,660,661,662,663,664,665,666,667,668,669,670,671,672,673,674,675,676,677,678,679,680,681,682,683,684,685,686,687,688,689,690,691,692,693,694,695,696,697,698,699,700,701,702,703,704,705,706,707,708,709,710,711,712,713,714,715,716,717,718,719,720,721,722,723,724,725,726,727,728,729,730,731,732,733,734,735,736,737,738,739,740,741,742,743,744,745,746,747,748,749,750,751,752,753,754,755,756,757,758,759,760,761,762,763,764,765,766,767,768,769,770,771,772,773,774,775,776,777,778,779,780,781,782,783,784,785,786,787,788,789,790,791,792,793,794,795,796,797,798,799,800,801,802,803,804,805,806,807,808,809,810,811,812,813,814,815,816,817,818,819,820,821,822,823,824,825,826,827,828,829,830,831,832,833,834,835,836,837,838,839,840,841,842,843,844,845,846,847,848,849,850,851,852,853,854,855,856,857,858,859,860,861,862,863,864,865,866,867,868,869,870,871,872,873,874,875,876,877,878,879,880,881,882,883,884,885,886,887,888,889,890,891,892,893,894,895,896,897,898,899,900,901,902,903,904,905,906,907,908,909,910,911,912,913,914,915,916,917,918,919,920,921,922,923,924,925,926,927,928,929,930,931,932,933,934,935,936,937,938,939,940,941,942,943,944,945,946,947,948,949,950,951,952,953,954,955,956,957,958,959,960,961,962,963,964,965,966,967,968,969,970,971,972,973,974,975,976,977,978,979,980,981,982,983,984,985,986,987,988,989,990,991,992,993,994,995,996,997,998,999,1000,1001,1002,1003,1004,1005,1006,1007,1008,1009,1010,1011,1012,1013,1014,1015,1016,1017,1018,1019,1020,1021,1022,1023,1024,1025,1026,1027,1028,1029,1030,1031,1032,1033,1034,1035,1036,1037,1038,1039,1040,1041,1042,1043,1044,1045,1046,1047,1048,1049,1050,1051,1052,1053,1054,1055,1056,1057,1058,1059,1060,1061,1062,1063,1064,1065,1066,1067,1068,1069,1070,1071,1072,1073,1074,1075,1076,1077,1078,1079,1080,1081,1082,1083,1084,1085,1086,1087,1088,1089,1090,1091,1092,1093,1094,1095,1096,1097,1098,1099,1100,1101,1102,1103,1104,1105,1106,1107,1108,1109,1110,1111,1112,1113,1114,1115,1116,1117,1118,1119,1120,1121,1122,1123,1124,1125,1126,1127,1128,1129,1130,1131,1132,1133,1134,1135,1136,1137,1138,1139,1140,1141,1142,1143,1144,1145,1146,1147,1148,1149,1150,1151,1152,1153,1154,1155,1156,1157,1158,1159,1160,1161,1162,1163,1164,1165,1166,1167,1168,1169,1170,1171,1172,1173,1174,1175,1176,1177,1178,1179,1180,1181,1182,1183,1184,1185,1186,1187,1188,1189,1190,1191,1192,1193,1194,1195,1196,1197,1198,1199,1200,1201,1202,1203,1204,1205,1206,1207,1208,1209,1210,1211,1212,1213,1214,1215,1216,1217,1218,1219,122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0,4221,4222,4223,4224,4225,4226,4227,4228,4229,4230,4231,4232,4233,4234,4235,4236,4237,4238,4239,4240,4241,4242,4243,4244,4245,4246,4247,4248,4249,4250,4251,4252,4253,4254,4255,4256,4257,4258,4259,4260,4261,4262,4263,4264,4265,4266,4267,4268,4269,4270,4271,4272,4273,4274,4275,4276,4277,4278,4279,4280,4281,4282,4283,4284,4285,4286,4287,4288,4289,4290,4291,4292,4293,4294,4295,4296,4297,4298,4299,4300,4301,4302,4303,4304,4305,4306,4307,4308,4309,4310,4311,4312,4313,4314,4315,4316,4317,4318,4319,4320,4321,4322,4323,4324,4325,4326,4327,4328,4329,4330,4331,4332,4333,4334,4335,4336,4337,4338,4339,4340,4341,4342,4343,4344,4345,4346,4347,4348,4349,4350,4351,4352,4353,4354,4355,4356,4357,4358,4359,4360,4361,4362,4363,4364,4365,4366,4367,4368,4369,4370,4371,4372,4373,4374,4375,4376,4377,4378,4379,4380,4381,4382,4383,4384,4385,4386,4387,4388,4389,4390,4391,4392,4393,4394,4395,4396,4397,4398,4399,4400,4401,4402,4403,4404,4405,4406,4407,4408,4409,4410,4411,4412,4413,4414,4415,4416,4417,4418,4419,4420,4421,4422,4423,4424,4425,4426,4427,4428,4429,4430,4431,4432,4433,4434,4435,4436,4437,4438,4439,4440,4441,4442,4443,4444,4445,4446,4447,4448,4449,4450,4451,4452,4453,4454,4455,4456,4457,4458,4459,4460,4461,4462,4463,4464,4465,4466,4467,4468,4469,4470,4471,4472,4473,4474,4475,4476,4477,4478,4479,4480,4481,4482,4483,4484,4485,4486,4487,4488,4489,4490,4491,4492,4493,4494,4495,4496,4497,4498,4499,4500,4501,4502,4503,4504,4505,4506,4507,4508,4509,4510,4511,4512,4513,4514,4515,4516,4517,4518,4519,4520,4521,4522,4523,4524,4525,4526,4527,4528,4529,4530,4531,4532,4533,4534,4535,4536,4537,4538,4539,4540,4541,4542,4543,4544,4545,4546,4547,4548,4549,4550,4551,4552,4553,4554,4555,4556,4557,4558,4559,4560,4561,4562,4563,4564,4565,4566,4567,4568,4569,4570,4571,4572,4573,4574,4575,4576,4577,4578,4579,4580,4581,4582,4583,4584,4585,4586,4587,4588,4589,4590,4591,4592,4593,4594,4595,4596,4597,4598,4599,4600,4601,4602,4603,4604,4605,4606,4607,4608,4609,4610,4611,4612,4613,4614,4615,4616,4617,4618,4619,4620,4621,4622,4623,4624,4625,4626,4627,4628,4629,4630,4631,4632,4633,4634,4635,4636,4637,4638,4639,4640,4641,4642,4643,4644,4645,4646,4647,4648,4649,4650,4651,4652,4653,4654,4655,4656,4657,4658,4659,4660,4661,4662,4663,4664,4665,4666,4667,4668,4669,4670,4671,4672,4673,4674,4675,4676,4677,4678,4679,4680,4681,4682,4683,4684,4685,4686,4687,4688,4689,4690,4691,4692,4693,4694,4695,4696,4697,4698,4699,4700,4701,4702,4703,4704,4705,4706,4707,4708,4709,4710,4711,4712,4713,4714,4715,4716,4717,4718,4719,4720,4721,4722,4723,4724,4725,4726,4727,4728,4729,4730,4731,4732,4733,4734,4735,4736,4737,4738,4739,4740,4741,4742,4743,4744,4745,4746,4747,4748,4749,4750,4751,4752,4753,4754,4755,4756,4757,4758,4759,4760,4761,4762,4763,4764,4765,4766,4767,4768,4769,4770,4771,4772,4773,4774,4775,4776,4777,4778,4779,4780,4781,4782,4783,4784,4785,4786,4787,4788,4789,4790,4791,4792,4793,4794,4795,4796,4797,4798,4799,4800,4801,4802,4803,4804,4805,4806,4807,4808,4809,4810,4811,4812,4813,4814,4815,4816,4817,4818,4819,4820,4821,4822,4823,4824,4825,4826,4827,4828,4829,4830,4831,4832,4833,4834,4835,4836,4837,4838,4839,4840,4841,4842,4843,4844,4845,4846,4847,4848,4849,4850,4851,4852,4853,4854,4855,4856,4857,4858,4859,4860,4861,4862,4863,4864,4865,4866,4867,4868,4869,4870,4871,4872,4873,4874,4875,4876,4877,4878,4879,4880,4881,4882,4883,4884,4885,4886,4887,4888,4889,4890,4891,4892,4893,4894,4895,4896,4897,4898,4899,4900,4901,4902,4903,4904,4905,4906,4907,4908,4909,4910,4911,4912,4913,4914,4915,4916,4917,4918,4919,4920,4921,4922,4923,4924,4925,4926,4927,4928,4929,4930,4931,4932,4933,4934,4935,4936,4937,4938,4939,4940,4941,4942,4943,4944,4945,4946,4947,4948,4949,4950,4951,4952,4953,4954,4955,4956,4957,4958,4959,4960,4961,4962,4963,4964,4965,4966,4967,4968,4969,4970,4971,4972,4973,4974,4975,4976,4977,4978,4979,4980,4981,4982,4983,4984,4985,4986,4987,4988,4989,4990,4991,4992,4993,4994,4995,4996,4997,4998,4999,5000,5001,5002,5003,5004,5005,5006,5007,5008,5009,5010,5011,5012,5013,5014,5015,5016,5017,5018,5019,5020,5021,5022,5023,5024,5025,5026,5027,5028,5029,5030,5031,5032,5033,5034,5035,5036,5037,5038,5039,5040,5041,5042,5043,5044,5045,5046,5047,5048,5049,5050,5051,5052,5053,5054,5055,5056,5057,5058,5059,5060,5061,5062,5063,5064,5065,5066,5067,5068,5069,5070,5071,5072,5073,5074,5075,5076,5077,5078,5079,5080,5081,5082,5083,5084,5085,5086,5087,5088,5089,5090,5091,5092,5093,5094,5095,5096,5097,5098,5099,5100,5101,5102,5103,5104,5105,5106,5107,5108,5109,5110,5111,5112,5113,5114,5115,5116,5117,5118,5119,5120,5121,5122,5123,5124,5125,5126,5127,5128,5129,5130,5131,5132,5133,5134,5135,5136,5137,5138,5139,5140,5141,5142,5143,5144,5145,5146,5147,5148,5149,5150,5151,5152,5153,5154,5155,5156,5157,5158,5159,5160,5161,5162,5163,5164,5165,5166,5167,5168,5169,5170,5171,5172,5173,5174,5175,5176,5177,5178,5179,5180,5181,5182,5183,5184,5185,5186,5187,5188,5189,5190,5191,5192,5193,5194,5195,5196,5197,5198,5199,5200,5201,5202,5203,5204,5205,5206,5207,5208,5209,5210,5211,5212,5213,5214,5215,5216,5217,5218,5219,5220,5221,5222,5223,5224,5225,5226,5227,5228,5229,5230,5231,5232,5233,5234,5235,5236,5237,5238,5239,5240,5241,5242,5243,5244,5245,5246,5247,5248,5249,5250,5251,5252,5253,5254,5255,5256,5257,5258,5259,5260,5261,5262,5263,5264,5265,5266,5267,5268,5269,5270,5271,5272,5273,5274,5275,5276,5277,5278,5279,5280,5281,5282,5283,5284,5285,5286,5287,5288,5289,5290,5291,5292,5293,5294,5295,5296,5297,5298,5299,5300,5301,5302,5303,5304,5305,5306,5307,5308,5309,5310,5311,5312,5313,5314,5315,5316,5317,5318,5319,5320,5321,5322,5323,5324,5325,5326,5327,5328,5329,5330,5331,5332,5333,5334,5335,5336,5337,5338,5339,5340,5341,5342,5343,5344,5345,5346,5347,5348,5349,5350,5351,5352,5353,5354,5355,5356,5357,5358,5359,5360,5361,5362,5363,5364,5365,5366,5367,5368,5369,5370,5371,5372,5373,5374,5375,5376,5377,5378,5379,5380,5381,5382,5383,5384,5385,5386,5387,5388,5389,5390,5391,5392,5393,5394,5395,5396,5397,5398,5399,5400,5401,5402,5403,5404,5405,5406,5407,5408,5409,5410,5411,5412,5413,5414,5415,5416,5417,5418,5419,5420,5421,5422,5423,5424,5425,5426,5427,5428,5429,5430,5431,5432,5433,5434,5435,5436,5437,5438,5439,5440
```

Relativistic Heavy Ion Collider Evaluation Software

Running Phenix regression tests

Author(s)

- - -

Purpose

The purpose of the regression tests are (one or always) to make in the Phenix code to make sure that the code is still working and something that is already added.

This regression tests can be used by users to make sure everything is working correctly.

Framework

Regression tests are located in many places in the Phenix and CTOW codebase. They are typically either in subdirectories called "regression_tests" or in files with a name ending in "_test". A list specified in a file which is the list can be anywhere in the CTOW codebase.

The regression tests are run by the "phenix.regression_test" program. This program will use the list of all the "list" files which are found when it is invoked in "phenix.cvs.list".

Running regression tests

You can run all the regression tests (usually on a machine with many processors) with a simple command:

```
phenix.regression_test -j 8 -v -t 600 -f
```

There are some simple keywords that you might want to add to this:

```
-v|--verbose Verbose: log the command and time
-j|--jobs=N  Number of jobs to run in parallel (default is the get
             processor count)
-t|--timeout=SECS Time out after SECS seconds (default 300)
-f|--force-run  Run the tests even if the cache says they ran in the
                last 24 hours
```

These keywords can be combined:

```
phenix.regression_test.py[exe|bat] -j[n|auto] -v[v] -t[n|n,n] [-f|-ff]
```

Python-based Macromolecular Crystallography

Remove test set reflections from a map file with remove_free_from_map

Author(s)

- Nicholas Free from_map Tom Terwilliger

Purpose

remove_free_from_map is a tool to remove test set reflections from a map coefficients file so that the map can be used in refinement without contamination from the test set reflections.

NOTE: Normally running this tool is unnecessary because most programs, including phenix.refine, ignore test set reflections in the input map.

Usage

How remove_free_from_map works:

remove_free_from_map reads in a set of map coefficients and:

Output files from remove_free_from_map

map_with_without_free_set.mtz An MTZ file with test set reflections set to 0+0

Examples

Standard run of remove_free_from_map:

Running remove_free_from_map is easy. From the command line you can type:

```
phenix.remove_free_from_map map_with_all.mtz free_1.mtz
```

remove_free_from_map uses Fourier, Bayes interpolation which reflections are in the test set.

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

Removing protein chains built into RNA density with remove_poor_fragments

Author(s):

- Andrew_poor_fragments: Tom Terwilliger

Purpose

Remove poorly-ordered chains that contains RNA and protein and tries to identify fragments of protein that were incorrectly built into RNA density.

Usage

Remove poorly-ordered chains that contains RNA and protein and tries to identify fragments of protein that were incorrectly built into RNA density.

How remove_poor_fragments works:

The main idea in this approach is that these incorrectly built chains tend to be oriented not in the trending of a protein backbone and to have lower map model correlations than the correct parts of the protein chains. The approach is to remove poorly-ordered chains that contain RNA and protein and to try to identify fragments of protein that are in correct phase in the trending of backbone and RNA residues in the chains that were not removed. The fragments are identified by looking for CA atoms that are close to RNA residues.

Keywords: AI, Artificial Intelligence, Machine Learning, Deep Learning, Neural Network

Description: Remove poorly-ordered chains that contain RNA and protein. Identify fragments of protein that are in correct phase in the trending of backbone and RNA residues in the chains that were not removed. Fragments are identified by looking for CA atoms that are close to RNA residues.

Comments: This approach is based on the idea that incorrectly built chains tend to be oriented not in the trending of a protein backbone and to have lower map model correlations than the correct parts of the protein chains. The approach is to remove poorly-ordered chains that contain RNA and protein and to try to identify fragments of protein that are in correct phase in the trending of backbone and RNA residues in the chains that were not removed. The fragments are identified by looking for CA atoms that are close to RNA residues.

Comments for the phenix.refine & phenix.autobuild interface: Input model and map are required. Output model is the input model with the fragments identified in the number of chains specified by the parameter chains_to_keep_in_output. Output map is the input map multiplied by a mask that is 1 in the vicinity of the fragments identified and 0 elsewhere. Output sequence file is the input sequence file minus the number of residues in the fragments identified.

Comments for the phenix.remove_poor_fragments command line interface: Input model and map are required. Output model is the input model with the fragments identified in the number of chains specified by the parameter chains_to_keep_in_output. Output map is the input map multiplied by a mask that is 1 in the vicinity of the fragments identified and 0 elsewhere. Output sequence file is the input sequence file minus the number of residues in the fragments identified.

Output files from remove_poor_fragments

Output_pdb.pdb: A PDB file with your minimal model

Output_seq.seq: A PDB file with your minimal model

Example

Running remove_poor_fragments is easy. From the command line you can type:

```
phenix.remove_poor_fragments model_pdb=input_pdb.pdb map_in=input_map.ccp4
```

Possible Problems

Specific limitations and problems:

Literature

Additional information

List of all available keywords:

model_pdb	input PDB file
map_in(MTZ_in)	Input map
map_out(MTZ_out)	Output map
output_pdb(PDB_out)	Output file name
seq_file_name	Sequence file name
output_seq(SEQ_out)	Output sequence file name
cutoff_factor	Cutoff factor for CA atoms near RNA to be removed (default 0.5)
chains_to_keep_in_output	Number of chains to keep in output (default all)
chain_id	Chain ID to be used for fragments (default A)
chain_type	Chain type to be used for fragments (PROTEIN or RNA/DNA)
n_cycles_to_check	Number of cycles to check for fragments (default 1)
n_residues_to_check	Number of residues to check for fragments (default 10)
n_residues_to_add	Number of residues to add to fragments (default 0)
n_residues_to_remove	Number of residues to remove from fragments (default 0)
n_residues_per_chain	Number of residues per chain to divide the main chain into (default 100)
n_cycles_to_refine	Number of cycles of refinement (default 0)
n_iter_to_remove	Number of iterations of removal of poorly-ordered chains (default 1)
n_protein_to_remove	Number of protein residues of poorly-ordered chains to remove (default 0)
n_rna_to_remove	Number of RNA/DNA residues of poorly-ordered chains to remove (default 0)
rna_only	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_<	Keep protein chains if number of protein residues < this (default 0)
remove_poor_fragments	Remove poorly-ordered chains that contain RNA and protein and try to identify fragments of protein that are in correct phase in the trending of backbone and RNA residues in the chains that were not removed. The fragments are identified by looking for CA atoms that are close to RNA residues. (default Yes)
remove_rna_chains	Remove all RNA/DNA chains (default No)
remove_protein_chains	Remove all protein chains (default No)
keep_rna_chains	Keep all RNA/DNA chains (default No)
keep_protein_chains	Keep all protein chains (default No)
n_residues_per_fragment	Number of residues per fragment (default 10)
n_fragments_per_chain	Number of fragments per chain (default 1)
n_cycles_to_refine_fragments	Number of cycles of refinement of fragments (default 0)
n_iter_to_remove_fragments	Number of iterations of removal of fragments (default 1)
n_protein_to_remove_fragments	Number of protein residues of fragments to remove (default 0)
n_rna_to_remove_fragments	Number of RNA/DNA residues of fragments to remove (default 0)
rna_only_fragments	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_fragments_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_fragments_<	Keep protein chains if number of protein residues < this (default 0)
remove_rna_chains_fragments	Remove all RNA/DNA chains (default No)
remove_protein_chains_fragments	Remove all protein chains (default No)
keep_rna_chains_fragments	Keep all RNA/DNA chains (default No)
keep_protein_chains_fragments	Keep all protein chains (default No)
n_iter_to_remove_fragments_fragments	Number of iterations of removal of fragments (default 1)
n_protein_to_remove_fragments_fragments	Number of protein residues of fragments to remove (default 0)
n_rna_to_remove_fragments_fragments	Number of RNA/DNA residues of fragments to remove (default 0)
rna_only_fragments_fragments	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_fragments_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_fragments_fragments_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_fragments_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_fragments_fragments_<	Keep protein chains if number of protein residues < this (default 0)
remove_rna_chains_fragments_fragments	Remove all RNA/DNA chains (default No)
remove_protein_chains_fragments_fragments	Remove all protein chains (default No)
keep_rna_chains_fragments_fragments	Keep all RNA/DNA chains (default No)
keep_protein_chains_fragments_fragments	Keep all protein chains (default No)
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
n_cycles	Number of cycles to run
n_iter_to_check	Number of iterations to check
n_iter_to_remove	Number of iterations to remove
n_residues_to_check	Number of residues to check
n_residues_to_add	Number of residues to add
n_residues_to_remove	Number of residues to remove
n_residues_per_chain	Number of residues per chain
n_cycles_to_refine	Number of cycles of refinement
n_iter_to_remove	Number of iterations of removal
n_protein_to_remove	Number of protein residues to remove
n_rna_to_remove	Number of RNA/DNA residues to remove
rna_only	Only RNA/DNA chains
keep_rna_chains_if_n_r_>	Keep RNA/DNA chains if number of RNA/DNA residues > this
keep_protein_chains_if_n_>	Keep protein chains if number of protein residues > this
keep_rna_chains_if_n_r_<	Keep RNA/DNA chains if number of RNA/DNA residues < this
keep_protein_chains_if_n_<	Keep protein chains if number of protein residues < this
remove_rna_chains	Remove all RNA/DNA chains
remove_protein_chains	Remove all protein chains
keep_rna_chains	Keep all RNA/DNA chains
keep_protein_chains	Keep all protein chains
n_residues_per_fragment	Number of residues per fragment
n_fragments_per_chain	Number of fragments per chain
n_cycles_to_refine_fragments	Number of cycles of refinement of fragments
n_iter_to_remove_fragments	Number of iterations of removal of fragments
n_protein_to_remove_fragments	Number of protein residues of fragments to remove
n_rna_to_remove_fragments	Number of RNA/DNA residues of fragments to remove
rna_only_fragments	Only RNA/DNA chains
keep_rna_chains_if_n_r_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this
keep_protein_chains_if_n_fragments_>	Keep protein chains if number of protein residues > this
keep_rna_chains_if_n_r_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this
keep_protein_chains_if_n_fragments_<	Keep protein chains if number of protein residues < this
remove_rna_chains_fragments	Remove all RNA/DNA chains
remove_protein_chains_fragments	Remove all protein chains
keep_rna_chains_fragments	Keep all RNA/DNA chains
keep_protein_chains_fragments	Keep all protein chains
n_iter_to_remove_fragments_fragments	Number of iterations of removal of fragments
n_protein_to_remove_fragments_fragments	Number of protein residues of fragments to remove
n_rna_to_remove_fragments_fragments	Number of RNA/DNA residues of fragments to remove
rna_only_fragments_fragments	Only RNA/DNA chains
keep_rna_chains_if_n_r_fragments_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this
keep_protein_chains_if_n_fragments_fragments_>	Keep protein chains if number of protein residues > this
keep_rna_chains_if_n_r_fragments_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this
keep_protein_chains_if_n_fragments_fragments_<	Keep protein chains if number of protein residues < this
remove_rna_chains_fragments_fragments	Remove all RNA/DNA chains
remove_protein_chains_fragments_fragments	Remove all protein chains
keep_rna_chains_fragments_fragments	Keep all RNA/DNA chains
keep_protein_chains_fragments_fragments	Keep all protein chains
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
n_cycles	Number of cycles to run
n_iter_to_check	Number of iterations to check
n_iter_to_remove	Number of iterations to remove
n_residues_to_check	Number of residues to check
n_residues_to_add	Number of residues to add
n_residues_to_remove	Number of residues to remove
n_residues_per_chain	Number of residues per chain
n_cycles_to_refine	Number of cycles of refinement
n_iter_to_remove	Number of iterations of removal
n_protein_to_remove	Number of protein residues to remove
n_rna_to_remove	Number of RNA/DNA residues to remove
rna_only	Only RNA/DNA chains
keep_rna_chains_if_n_r_>	Keep RNA/DNA chains if number of RNA/DNA residues > this
keep_protein_chains_if_n_>	Keep protein chains if number of protein residues > this
keep_rna_chains_if_n_r_<	Keep RNA/DNA chains if number of RNA/DNA residues < this
keep_protein_chains_if_n_<	Keep protein chains if number of protein residues < this
remove_rna_chains	Remove all RNA/DNA chains
remove_protein_chains	Remove all protein chains
keep_rna_chains	Keep all RNA/DNA chains
keep_protein_chains	Keep all protein chains
n_residues_per_fragment	Number of residues per fragment
n_fragments_per_chain	Number of fragments per chain
n_cycles_to_refine_fragments	Number of cycles of refinement of fragments
n_iter_to_remove_fragments	Number of iterations of removal of fragments
n_protein_to_remove_fragments	Number of protein residues of fragments to remove
n_rna_to_remove_fragments	Number of RNA/DNA residues of fragments to remove
rna_only_fragments	Only RNA/DNA chains
keep_rna_chains_if_n_r_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this
keep_protein_chains_if_n_fragments_>	Keep protein chains if number of protein residues > this
keep_rna_chains_if_n_r_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this
keep_protein_chains_if_n_fragments_<	Keep protein chains if number of protein residues < this
remove_rna_chains_fragments	Remove all RNA/DNA chains
remove_protein_chains_fragments	Remove all protein chains
keep_rna_chains_fragments	Keep all RNA/DNA chains
keep_protein_chains_fragments	Keep all protein chains
n_iter_to_remove_fragments_fragments	Number of iterations of removal of fragments
n_protein_to_remove_fragments_fragments	Number of protein residues of fragments to remove
n_rna_to_remove_fragments_fragments	Number of RNA/DNA residues of fragments to remove
rna_only_fragments_fragments	Only RNA/DNA chains
keep_rna_chains_if_n_r_fragments_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this
keep_protein_chains_if_n_fragments_fragments_>	Keep protein chains if number of protein residues > this
keep_rna_chains_if_n_r_fragments_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this
keep_protein_chains_if_n_fragments_fragments_<	Keep protein chains if number of protein residues < this
remove_rna_chains_fragments_fragments	Remove all RNA/DNA chains
remove_protein_chains_fragments_fragments	Remove all protein chains
keep_rna_chains_fragments_fragments	Keep all RNA/DNA chains
keep_protein_chains_fragments_fragments	Keep all protein chains
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
chain_id	Chain ID to be used for fragments (default A)
chain_type	Chain type to be used for fragments (PROTEIN or RNA/DNA)
cutoff_factor	Cutoff factor for CA atoms near RNA to be removed (default 0.5)
n_cycles_to_check	Number of cycles to check for fragments (default 1)
n_residues_to_check	Number of residues to check for fragments (default 10)
n_residues_to_add	Number of residues to add to fragments (default 0)
n_residues_to_remove	Number of residues to remove from fragments (default 0)
n_residues_per_chain	Number of residues per chain to divide the main chain into (default 100)
n_cycles_to_refine	Number of cycles of refinement (default 0)
n_iter_to_remove	Number of iterations of removal of poorly-ordered chains (default 1)
n_protein_to_remove	Number of protein residues of poorly-ordered chains to remove (default 0)
n_rna_to_remove	Number of RNA/DNA residues of poorly-ordered chains to remove (default 0)
rna_only	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_<	Keep protein chains if number of protein residues < this (default 0)
remove_poor_fragments	Remove poorly-ordered chains that contain RNA and protein and try to identify fragments of protein that are in correct phase in the trending of backbone and RNA residues in the chains that were not removed. The fragments are identified by looking for CA atoms that are close to RNA residues. (default Yes)
remove_rna_chains	Remove all RNA/DNA chains (default No)
remove_protein_chains	Remove all protein chains (default No)
keep_rna_chains	Keep all RNA/DNA chains (default No)
keep_protein_chains	Keep all protein chains (default No)
n_residues_per_fragment	Number of residues per fragment (default 10)
n_fragments_per_chain	Number of fragments per chain (default 1)
n_cycles_to_refine_fragments	Number of cycles of refinement of fragments (default 0)
n_iter_to_remove_fragments	Number of iterations of removal of fragments (default 1)
n_protein_to_remove_fragments	Number of protein residues of fragments to remove (default 0)
n_rna_to_remove_fragments	Number of RNA/DNA residues of fragments to remove (default 0)
rna_only_fragments	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_fragments_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_fragments_<	Keep protein chains if number of protein residues < this (default 0)
remove_rna_chains_fragments	Remove all RNA/DNA chains (default No)
remove_protein_chains_fragments	Remove all protein chains (default No)
keep_rna_chains_fragments	Keep all RNA/DNA chains (default No)
keep_protein_chains_fragments	Keep all protein chains (default No)
n_iter_to_remove_fragments_fragments	Number of iterations of removal of fragments (default 1)
n_protein_to_remove_fragments_fragments	Number of protein residues of fragments to remove (default 0)
n_rna_to_remove_fragments_fragments	Number of RNA/DNA residues of fragments to remove (default 0)
rna_only_fragments_fragments	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_fragments_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_fragments_fragments_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_fragments_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_fragments_fragments_<	Keep protein chains if number of protein residues < this (default 0)
remove_rna_chains_fragments_fragments	Remove all RNA/DNA chains (default No)
remove_protein_chains_fragments_fragments	Remove all protein chains (default No)
keep_rna_chains_fragments_fragments	Keep all RNA/DNA chains (default No)
keep_protein_chains_fragments_fragments	Keep all protein chains (default No)
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
chains_to_keep_in_output	Number of chains to keep in output (default all)
chain_id	Chain ID to be used for fragments (default A)
chain_type	Chain type to be used for fragments (PROTEIN or RNA/DNA)
cutoff_factor	Cutoff factor for CA atoms near RNA to be removed (default 0.5)
n_cycles_to_check	Number of cycles to check for fragments (default 1)
n_residues_to_check	Number of residues to check for fragments (default 10)
n_residues_to_add	Number of residues to add to fragments (default 0)
n_residues_to_remove	Number of residues to remove from fragments (default 0)
n_residues_per_chain	Number of residues per chain to divide the main chain into (default 100)
n_cycles_to_refine	Number of cycles of refinement (default 0)
n_iter_to_remove	Number of iterations of removal of poorly-ordered chains (default 1)
n_protein_to_remove	Number of protein residues of poorly-ordered chains to remove (default 0)
n_rna_to_remove	Number of RNA/DNA residues of poorly-ordered chains to remove (default 0)
rna_only	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_<	Keep protein chains if number of protein residues < this (default 0)
remove_rna_chains	Remove all RNA/DNA chains (default No)
remove_protein_chains	Remove all protein chains (default No)
keep_rna_chains	Keep all RNA/DNA chains (default No)
keep_protein_chains	Keep all protein chains (default No)
n_residues_per_fragment	Number of residues per fragment (default 10)
n_fragments_per_chain	Number of fragments per chain (default 1)
n_cycles_to_refine_fragments	Number of cycles of refinement of fragments (default 0)
n_iter_to_remove_fragments	Number of iterations of removal of fragments (default 1)
n_protein_to_remove_fragments	Number of protein residues of fragments to remove (default 0)
n_rna_to_remove_fragments	Number of RNA/DNA residues of fragments to remove (default 0)
rna_only_fragments	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_fragments_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_fragments_<	Keep protein chains if number of protein residues < this (default 0)
remove_rna_chains_fragments	Remove all RNA/DNA chains (default No)
remove_protein_chains_fragments	Remove all protein chains (default No)
keep_rna_chains_fragments	Keep all RNA/DNA chains (default No)
keep_protein_chains_fragments	Keep all protein chains (default No)
n_iter_to_remove_fragments_fragments	Number of iterations of removal of fragments (default 1)
n_protein_to_remove_fragments_fragments	Number of protein residues of fragments to remove (default 0)
n_rna_to_remove_fragments_fragments	Number of RNA/DNA residues of fragments to remove (default 0)
rna_only_fragments_fragments	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_fragments_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_fragments_fragments_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_fragments_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_fragments_fragments_<	Keep protein chains if number of protein residues < this (default 0)
remove_rna_chains_fragments_fragments	Remove all RNA/DNA chains (default No)
remove_protein_chains_fragments_fragments	Remove all protein chains (default No)
keep_rna_chains_fragments_fragments	Keep all RNA/DNA chains (default No)
keep_protein_chains_fragments_fragments	Keep all protein chains (default No)
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
chains_to_keep_in_output	Number of chains to keep in output (default all)
chain_id	Chain ID to be used for fragments (default A)
chain_type	Chain type to be used for fragments (PROTEIN or RNA/DNA)
cutoff_factor	Cutoff factor for CA atoms near RNA to be removed (default 0.5)
n_cycles_to_check	Number of cycles to check for fragments (default 1)
n_residues_to_check	Number of residues to check for fragments (default 10)
n_residues_to_add	Number of residues to add to fragments (default 0)
n_residues_to_remove	Number of residues to remove from fragments (default 0)
n_residues_per_chain	Number of residues per chain to divide the main chain into (default 100)
n_cycles_to_refine	Number of cycles of refinement (default 0)
n_iter_to_remove	Number of iterations of removal of poorly-ordered chains (default 1)
n_protein_to_remove	Number of protein residues of poorly-ordered chains to remove (default 0)
n_rna_to_remove	Number of RNA/DNA residues of poorly-ordered chains to remove (default 0)
rna_only	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_<	Keep protein chains if number of protein residues < this (default 0)
remove_rna_chains	Remove all RNA/DNA chains (default No)
remove_protein_chains	Remove all protein chains (default No)
keep_rna_chains	Keep all RNA/DNA chains (default No)
keep_protein_chains	Keep all protein chains (default No)
n_residues_per_fragment	Number of residues per fragment (default 10)
n_fragments_per_chain	Number of fragments per chain (default 1)
n_cycles_to_refine_fragments	Number of cycles of refinement of fragments (default 0)
n_iter_to_remove_fragments	Number of iterations of removal of fragments (default 1)
n_protein_to_remove_fragments	Number of protein residues of fragments to remove (default 0)
n_rna_to_remove_fragments	Number of RNA/DNA residues of fragments to remove (default 0)
rna_only_fragments	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_fragments_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_fragments_<	Keep protein chains if number of protein residues < this (default 0)
remove_rna_chains_fragments	Remove all RNA/DNA chains (default No)
remove_protein_chains_fragments	Remove all protein chains (default No)
keep_rna_chains_fragments	Keep all RNA/DNA chains (default No)
keep_protein_chains_fragments	Keep all protein chains (default No)
n_iter_to_remove_fragments_fragments	Number of iterations of removal of fragments (default 1)
n_protein_to_remove_fragments_fragments	Number of protein residues of fragments to remove (default 0)
n_rna_to_remove_fragments_fragments	Number of RNA/DNA residues of fragments to remove (default 0)
rna_only_fragments_fragments	Only RNA/DNA chains (default No)
keep_rna_chains_if_n_r_fragments_fragments_>	Keep RNA/DNA chains if number of RNA/DNA residues > this (default 0)
keep_protein_chains_if_n_fragments_fragments_>	Keep protein chains if number of protein residues > this (default 0)
keep_rna_chains_if_n_r_fragments_fragments_<	Keep RNA/DNA chains if number of RNA/DNA residues < this (default 0)
keep_protein_chains_if_n_fragments_fragments_<	Keep protein chains if number of protein residues < this (default 0)
remove_rna_chains_fragments_fragments	Remove all RNA/DNA chains (default No)
remove_protein_chains_fragments_fragments	Remove all protein chains (default No)
keep_rna_chains_fragments_fragments	Keep all RNA/DNA chains (default No)
keep_protein_chains_fragments_fragments	Keep all protein chains (default No)
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)
output_dir	Output directory
overwrite	Overwrite existing files (default Yes)
verbose	Verbose output (default No)
debug	Debugging output (default No)
nproc	Number of processors (default 1)
output_prefix	Prefix for output files
output_suffix	Suffix for output files
output_extension	Extension for output files
write_log_file	Write a log file (default No)
log_extension	Extension for log file
write_parameters	Write parameters to file (default No)

Phasta — Python Sequence Analysis Modules for Integrated Bioinformatics

phasta.remember_fab

Description

The remember_fab module is designed to streamline the concatenating process for FASTA files. It performs a search through all of FASTA sequences in the fasta file, and when sequence whose identifier (its sequence is set to be the first line of the sequence, up to the first space or tab) matches the specified identifier, it writes it to stdout. Unlike, and faster, than the fasta_grep.

Given a list of identifiers, it will write the corresponding sequence.

Ensure that the sequence encompasses the entire PAS structure and adequately covers the entire chains in the complex.

Alternatively, the tool will update HELIXSHAPE-formatted records describing secondary structure. However, it will neither recompute the output HSAPRED, CSPR, and ancient union records.

You can customize the similarity threshold by adjusting the flanking nucleotides in case the sequences are not identical. The default setting requires an exact match for the sequence and identifier.

[NOTICE] The program work against sequence in Bitbucket server at https://bitbucket.org/phasta/phasta. Please acknowledge the server activity. Bitbucket.org, Atlassian, Inc. Atlassian, 1098 Harrison Street, San Francisco, CA 94103, https://www.atlassian.com/about

Command line usage examples

```
% phasta.remember_fab input.pdb sequence.fa
```

To phasta.remember_fab input.pdb sequence.fa

```
% phasta.remember_fab -id sequence.fa sometimes-shortlong-identity-id.fa
```

Keywords

Keywords available in the Phasta GUI in the "FAB Assembler" section:

List of all available keywords

```
OUTMAX = <DEFAULT CONTROL DEFAULT>          ALLOW OLDMAX TO LIM
OUTMAX = <LIM>                              MATCH THE EXACT
IDENTITY=<DEFAULT 0.5>                      MATCH THE FIRST WORD OF THE FASTA HEADER (TO LIFT THE
                                            SEQUENCE FROM THE FASTA FILE FOR ALIGNMENT OR SUBMITTING
                                            TO SERVERS)
IDENTITY = <Num>                            MAX TITLE LENGTH MUST NOT EXCEED LENGTH LIM
                                            (DEFAULT 255)
                                            ALLOW FILE-NAMES AS OUTPUTS(ALL OUTPUT FILENAMES, IF
                                            NOT SPECIFIED, DEFAULT TO STDOUT)
                                            PDB-SEQRES-ADDRESS: PREFIX TO ADDRESS DIRECTORY
OUTPUT = <Name>
OUTPUT2 = <Name>
OUTPUT3 = <Name>
OUTPUT4 = <Name>
OUTPUT5 = <Name>
OUTPUT6 = <Name>
OUTPUT7 = <Name>
OUTPUT8 = <Name>
OUTPUT9 = <Name>
OUTPUT10 = <Name>
OUTPUT11 = <Name>
OUTPUT12 = <Name>
OUTPUT13 = <Name>
OUTPUT14 = <Name>
OUTPUT15 = <Name>
OUTPUT16 = <Name>
OUTPUT17 = <Name>
OUTPUT18 = <Name>
OUTPUT19 = <Name>
OUTPUT20 = <Name>
OUTPUT21 = <Name>
OUTPUT22 = <Name>
OUTPUT23 = <Name>
OUTPUT24 = <Name>
OUTPUT25 = <Name>
OUTPUT26 = <Name>
OUTPUT27 = <Name>
OUTPUT28 = <Name>
OUTPUT29 = <Name>
OUTPUT30 = <Name>
OUTPUT31 = <Name>
OUTPUT32 = <Name>
OUTPUT33 = <Name>
OUTPUT34 = <Name>
OUTPUT35 = <Name>
OUTPUT36 = <Name>
OUTPUT37 = <Name>
OUTPUT38 = <Name>
OUTPUT39 = <Name>
OUTPUT40 = <Name>
OUTPUT41 = <Name>
OUTPUT42 = <Name>
OUTPUT43 = <Name>
OUTPUT44 = <Name>
OUTPUT45 = <Name>
OUTPUT46 = <Name>
OUTPUT47 = <Name>
OUTPUT48 = <Name>
OUTPUT49 = <Name>
OUTPUT50 = <Name>
```

PHENIX *Python-based Hierarchical Environment for Integrated Xtallography*

Replace side chains in a model to match the sequence with replace_side_chains

Author(s):

- Pavel Afonine, Oleg V. Sobolev

Purpose:

Replace side chains in a model to match a given map model and to add side chains from a rotamer library based on an electron density map.

Note: the rotamer library is called from phenix.phase_and_build but you can use it interactively if you want.

Note: the program requires a map (separate) from a model (without side chains (or with) and a map (with sequence from density).

Usage

How replace_side_chains works:

replace_side_chains works in order to replace the side chains as needed. You can choose to use the default rotamer library or provide your own rotamer library.

Output files from replace_side_chains

replace_side_chains.pdb: A PDB file with side chains replaced

Examples

Standard run of replace_side_chains:

Running replace_side_chains is easy. Find the commands line you can type:

phenix.replace_side_chains -h | more (to see the help message)

You should supply a sequence file that contains the sequence of the model.

Using replace_side_chains to sequence a protein from density:

From the command line you can type:

phenix.replace_side_chains model.pdb map.ccp4***

Possible Problems

Specific limitations and problems:

Literature

Additional information

Phenix *Python-based Hierarchical Environment for Integrated Bioinformatics*

Rebuild a model using fragments from the PDB

Author(s)

Tom Terwilliger, Pavel Afonine, Oleg Sobolev

Purpose

Creates a complete model similar to a supplied model using fragments from the PDB.

This tool can be used in early stages of model building to try and improve parts of a preliminary model by replacing them with fragments from structures in the PDB.

Note that this procedure does not use the sequence from your structure, but rather generates the fragments that match the supplied model and also because the junctions between fragments taken from the PDB are not refined.

Usage

replace_with_fragments_from_pdb can create composite models for protein chains

You can specify the resolution for selection of fragments/molecules in each helix/strand/fragment and whether to include helices, strands, and other fragments in the model.

You can supply a map file for refinement or calculation of map model correlations.

You can ask phenix to execute a minute specific PDB searching and fragment searching, or you can supply a file with a list of PDB codes to use for fragments.

You can choose to create a bootstrapped fit and a refined part of your model (by supplying a selection string for the refined part).

New replace_with_fragments_from_pdb works:

replace_with_fragments_from_PDB finds PDB matching sequences and extracts the fragments similar to segments in supplied model. Then connects the extracted fragments to form part of the supplied model and creates a complete model from the fragments.

replace_with_fragments_from_pdb uses PDB-based secondary structure statistics to find structures in the PDB that are similar to the supplied model. Then it extracts the fragments and connects them together.

replace_with_fragments_from_pdb also uses fragment searching to find similar fragments matching each loop (segment between two helices or strands) in the supplied model.

The fragments found by the searches are then connected together and refined (bootstrap) to make the distance between starting and ending residues match the distance in the supplied structure.

Fragments detected from PDB searching are optionally resolved to match the target structure as well. The resolved fragments are then connected together and refined (bootstrap) to make the distance between starting and ending residues match the distance in the supplied structure.

The supplied model is then used as a template and combined with the set of pieces from the PDB and superimposed on the template. The best matching segments (smallest rmsd and longest length) are chosen and connected together to form the final model by Modeller/Fragment Assembly of the PDB.

Examples

Standard run of replace_with_fragments_from_pdb:

Running replace_with_fragments_from_pdb is easy. Find the command line you can type:

```
phenix.replace_with_fragments_from_pdb model.pdb sequence
```

Output from the program is the PDB similar to model.pdb, put them together and write out a new model using these fragments.

Possible Problems

Specific limitations and problems:

The final model may have poor geometry at connections between fragments, so further refinement is normally required. Also, the final model may have poor geometry where sequence between ends is similar but not match the target structure.

Literature

Additional information

List of all available keywords

```
input {
  pdb_file_name = None
  sequence = None
  map_file = None
  map_model
    .multiple = True
    .file_name = None
    .name = None
}
output
  .prefix_model = None
  .prefix_map = None
replace_with_fragments_from_pdb
  .verbose_level
    .type = int(value=0,-1,1,2,3)
    .help = Verbosity level
  .keep_ligands = keep_all_ligands
    .type = bool
    .help = Keep ligands in the PDB
  .max_search_hits = None
    .type = int(value=1,100000000)
    .help = Maximum number of hits to use
  .pdb_search_sequence = None
    .type = str
    .help = Sequence to use for PDB search
  .pdb_search_file = None
    .type = path
    .help = File with list of PDB codes to use
  .max_pdb_codes_to_fetch = None
    .type = int(value=1,100000000)
    .help = Maximum number of PDB codes to fetch
  .max_pdb_codes_to_fetch_per_hit = None
    .type = int(value=1,100000000)
    .help = Maximum number of PDB codes to fetch per hit
  .max_pdb_search_identity_to_ref_seq = None
    .type = int(value=0,100)
    .help = Maximum identity to reference PDB chain to include. Default
            is 100 (keep all). Lowering this will cause the
            fragments to be more different than the reference.
  .max_pdb_search_identity_to_fragment_seq = None
    .type = int(value=0,100)
    .help = Maximum identity to fragment PDB chain to include. Default
            is 100 (keep all). Lowering this will cause the fragment
            sequence to be more different than the reference.
  .fix_fragment_search_for_pdb_search = False
    .type = bool
    .help = Fix fragment search for pdb search and use the same hits
            for each fragment (instead of different hits for each
            fragment)
  .fragment_resolution = None
    .type = float(value=0.0,100.0)
    .help = Resolution of fragments
  .connecting_method = A_and_B_and_C
    .type = enum(A_and_B_and_C,A_or_B_or_C,A_or_B_or_C_or_D,A_or_B_or_
            C_or_D_or_E,A_or_B_or_C_or_D_or_E_or_F,A_or_B_or_C_or_D_or_E_
            or_F_or_G,A_or_B_or_C_or_D_or_E_or_F_or_G_or_H,A_or_B_or_C_or
            _D_or_E_or_F_or_G_or_H_or_I,A_or_B_or_C_or_D_or_E_or_F_or_G_or
            _H_or_I_or_J,A_or_B_or_C_or_D_or_E_or_F_or_G_or_H_or_I_or_J_or
            _K,A_or_B_or_C_or_D_or_E_or_F_or_G_or_H_or_I_or_J_or_K_or_L)
    .help = Method combining of seq
  .chain_length_for_fragment_search = None
    .type = int(value=1,100000000)
    .help = Length of chain to use for fragment searches. Default
            is 20 (use 20 residues for fragment searches). Lowering
            this will cause more hits to be found.
  .fix_chain_length_for_fragment_search = False
    .type = bool
    .help = Fix length of chain for fragment search (use the entire chain
            for each fragment search)
  .number_of_processors = None
    .type = int(value=1,100000000)
    .help = Number of processors (if Mpiru has all processors)
  .fix_fragments_connection_method = False
    .type = bool
    .help = Fix the method for connecting fragments (use the connection
            method specified in the connecting_method keyword) (default is
            try the best for connection)
  .output_dir = None
    .type = path
    .help = Output directory
  .debug = False
    .type = bool
    .help = Debugging parameter (keep temp files)
}
```

Phenix

Action-based Hierarchical Mechanism for Integrated Multiagents

Density modification of cryo EM maps with resolve_cryo_em

Author(s)

- Pavel V. Afonine, Tom Terwilliger

Purpose

The Phenix module _cryo_em_ is a tool for carrying out density modification of cryo-EM maps

Uses

Density modification with resolve_cryo_em is carried out using four half-maps, along with the FSC based information about the resolution and quality of the data.

Density modification with resolve_cryo_em can be used to carry out initial density modification (e.g. if half-map quality is poor) or to carry out density modification using the half-maps and information about the resolution and quality of the data to improve a cryo-EM map based density modified map.

Video Tutorial

The Phenix tutorial is available on the Phenix YouTube channel and covers the following topics:

- Data overview
- How to run resolve_cryo_em via the GUI

How resolve_cryo_em works:

Resolve_cryo_em carries out density modification using two maps. One is the half-map in Phenix unsharpened format (the half-map with the B-factor of the original map applied to it) and the other is the difference map between the two half-maps. The difference map is used to estimate the noise in the map, and the unsharpened half-map is used as a target map. Combined errors in the contract are those where one Fourier component in one half-map is not consistent with the other half-map.

The goal of the density modification is to carry out changes to a map that improve the agreement between the two half-maps, while also making changes that are consistent with the expected properties of a cryo-EM map (such as solvent flattening, histogram matching, etc).

The density modification procedure carries out a Fourier coefficient for the map was adjusted to agree both with the original half-map and with expected features. This procedure is iterative (coefficients and the map are recalculated and then the procedure is repeated) and is carried out using a variety of cycles and cycle types.

Unique features of density modification for cryo-EM are that two half-maps with independent errors are available and that information about resolution and quality of the data is available. Resolve_cryo_em makes use of this information in a variety of ways, including using it to estimate the noise in the map, to estimate the resolution, and to carry out cross-validation. Cross-validation is used to avoid overfitting.

Using resolve_cryo_em:

Resolve_cryo_em is available in the Phenix GUI (Phenix) and covers the following topics:

- Data overview
- How to run resolve_cryo_em via the GUI

How resolve_cryo_em works:

Resolve_cryo_em carries out density modification using two maps. One is the half-map in Phenix unsharpened format (the half-map with the B-factor of the original map applied to it) and the other is the difference map between the two half-maps. The difference map is used to estimate the noise in the map, and the unsharpened half-map is used as a target map. Combined errors in the contract are those where one Fourier component in one half-map is not consistent with the other half-map. The goal of the density modification is to carry out changes to a map that improve the agreement between the two half-maps, while also making changes that are consistent with the expected properties of a cryo-EM map (such as solvent flattening, histogram matching, etc).

local_pathmap_from_curr	false	Map pathmap from current to local
remote_pathmap_from	false	If remote pathmap, map remote pathmap prefix from a remote path to local path. Used when the remote machine has a different mount point than the local machine. Multiple mappings can be separated by commas.
checkpoint_type	Base Spot	Checkpoint type. Base checkpoints are created at the start of a job. Spot checkpoints are created when a spot instance is about to be terminated.
		Checkpoint spot wait. Amount of time to wait for a spot checkpoint to complete before terminating the instance. Checkpoints that do not complete within the specified time will be ignored. Specified in seconds. Default: 120
checkpoint_spot_wait	120	Checkpoint spot wait. Amount of time to wait for a spot checkpoint to complete before terminating the instance. Checkpoints that do not complete within the specified time will be ignored. Specified in seconds. Default: 120
		Checkpoint spot wait. Amount of time to wait for a spot checkpoint to complete before terminating the instance. Checkpoints that do not complete within the specified time will be ignored. Specified in seconds. Default: 120
cpifile		Checkpoint input file
debug	false	Debug of spot-ec2-run
disable_c_cache_management	yes,no,a,n,y,N	
		Disable cache management in many cycles, does not apply if
		Disable cache management in many cycles, does not apply if
force_cycle	true	Keep cycle if last cycle exec of an hour
disable_mem2mem_get_cycle	true	
		Disable mem2mem in many cycles, does not apply if debug is
		Disable mem2mem in many cycles, does not apply if debug is
only_half_between_cycle	false	
		Perform calculation between daily-weekday and weekend, or only
only_high_price	100	If set true, ignore, this option is only for Project, Inherit
ec2_id		Specify ec2 instance id to use, if not specified,
		Specify ec2 instance id to use, if not specified,
		Specify ec2 instance id to use, if not specified,
service_for_final_value	true	Instead of using the calculated value, use the service
max_in_service	0.5	Maximum fraction of the service instances that can be
		Maximum fraction of the service instances that can be
		Maximum fraction of the service instances that can be

Phenix *Python-based Hierarchical Environment for Integrated Xtallography*

General Installation Instructions for Rosetta for use in Phenix

Contents

- Installation
- Installation - Using standard Phenix installation
- Installation - Using
- Phenix Rosetta Setup
- Troubleshooting

Installation

Rosetta is software from the Baker laboratory at the University of Washington (https://www.rosettacommons.org). Rosetta is used by a number of modules in Phenix:

- phenix.rosetta_refine
- phenix.rosetta_fitmaps (crude)
- phenix.rosetta_adp

Phenix provides the rosetta a compilation of Rosetta from source as a binary (some exceptions for non-standard platforms) and Phenix provides the wrapper to the binary and Rosetta. This is a brief program of what is required to install Rosetta for use in Phenix. Please see the Rosetta Commons website for more information on making the effort to install the compiled version of Rosetta (means that you can run all phenix Rosetta dependent programs).

Once you have installed Rosetta you need to set the environmental variable PHENIX_ROSETTA_PATH.

Installation - Using standard Phenix installation

To use the new Rosetta service, Phenix needs to be installed using a version compatible with v1.11 onwards. The installation process will ask if you want to download the Rosetta binaries. Please read the installer and install Rosetta or get the binaries.

Rosetta binaries are available for Linux, macos, cygwin and mac(M-Dgit) Intel (10.12). The installer is currently only a step in the installation instructions is generating bugs that are using large amounts of memory.

Provided with the following:

- The Rosetta Commons website and Phenix binaries(note there is get a license and then to download Rosetta). Rosetta binaries are provided as .tar files. It is quicker to download the source Rosetta. The binaries are separate when installing for ALL programs.
- Make a directory for Rosetta (Phenix will create a directory if does not already exist). Move the downloaded file into the directory and untar the file. Make sure you know where the Rosetta.
- Set environmental variable PHENIX_ROSETTA_PATH. Usually like this:
  - `setenv PHENIX_ROSETTA /path/to/rosetta`
- Make sure you have a directory file rosetta_db_2016.17.zxxx. Zxxxfile that contains:
  - `mkdir -p database/chemical/mm/charmm/`
- The directory containing "rosetta database" is set by either "PHENIX_ROSETTA_INPUT". Now you can now set environmental variable PHENIX_ROSETTA_INPUT to the path to "database". (setenv PHENIX_ROSETTA_INPUT /path/to/rosetta database). If you are using the latest set of whole.
  - `export PHENIX_ROSETTA_INPUT=/path/to/rosetta/database/`
  - `setenv PHENIX_ROSETTA_INPUT /path/to/rosetta/database/`
- unzip PHENIX_ROSETTA_PATH/zxxx.zipfile to rosetta.tar.
- The final step is to build the interface for rosetta. (phrix. It will also build Rosetta MoD if it is not done yet. Rosetta MoD is a set of Rosetta modules that are required for Phenix. Rosetta MoD is a set of Rosetta modules that are required for Phenix. Rosetta MoD is a set of Rosetta modules that are required for Phenix

Phenix

Python-based Hierarchical Environment for Integrated Xtallography

Crystallographic refinement with Rosetta (phenix.rosetta_refine)

Contents

- Overview
- Installation
- Execution
- Limitations
- Troubleshooting
- References
- List of all available keywords

Overview

The program phenix.rosetta_refine provides a convenient wrapper for running Rosetta reflinement of protein in low cryoEM resolution (Chiang et al. 2012), which integrates the Rosetta methods for conformational sampling and refinement with the Phenix crystallographic refinement and validation tools. Rosetta is a suite of C++ and MPI-based software for macromolecular structure prediction and design, including a flexible, object-oriented framework for protein modeling and sampling, and the capability to work directly with crystallographic data.

Currently both the setup and execution of Rosetta structural tasks are extensive, please read the entire documentation carefully before attempting to use this program. **Installation and validation has not yet Windows, you must have a Mac or Linux system to use this program.**

Installation

The Rosetta suite must be installed the appropriate version of Rosetta. The binary rosetta should be sufficient; users of the MPI version of Rosetta can set up the command-line accelerator with the command (assuming the version of Rosetta is 2.3.0):

```
setup.Rosetta(version=2.3.0,CONDA=/path/to/miniconda/envs/rosetta_env)
```

For developers of Rosetta, you must have installed Rosetta, software downloaded from the Rosetta laboratory at the University of Washington.

See the general installation notes for Rosetta

Execution

Running phenix.rosetta_refine is superficially similar to running phenix.refine, but with a much more limited set of parameters and output files. Rosetta refinement is a stochastic process, and it may be necessary to run multiple times. Phenix offers several procedures to help manage all simulations in one, the method for accomplishing this depends on the job scheduler on your computer or cluster.

```
phenix.rosetta_refine model.pdb data.mtz nproc=12 nstructures=100 output.prefix=test
```

This command will run up to 12 jobs at a time, and write a total of 100 refined structures, creating files test_001.pdb and test_001.mtz. The output files will be numbered in order from 1 and the output prefix defaults to refine but can be specified using the output.prefix keyword. If desired, the argument nproc=1 can be specified to run the jobs in series, or nproc=auto will attempt to determine the number of processors on the local machine.

The default parameterization strategy is between the "full" and "fast" protocols, both of which are described using the Rosetta2005 series (Chaudhury et al. 2011). The "fast" protocol is intended both for high-resolution structures and for cases where the input model is very close to the solution, and will generally be much faster than the "full" protocol. Both protocols use "low res mode" and use the same set of underlying energy functions, specified in phenix.rosetta.cfg.

You can use the program to parallelize jobs across multiple CPUs or several different queuing systems. The simplest method is multiprocessing on a single CPU, which is the default if nproc is greater than 1. The number of actual number of processors will be limited by the nproc=N argument, which defaults to 1. Depending on the number of processors available, the program will automatically choose between "fast" and "full" protocols if the difference of more than 2.0% in R-free.

Alternatively, you can specify the queuing system with "nproc=N", with the directory number increasing sequentially for additional runs (for example Phenix jobs.cfg is used as the final step, the output files are numbered from 1 to the number of jobs).

Limitations

The program has several restrictions compared to phenix.refine:

- Molecules are limited to the standard amino acids and a small number of cofactors and ions. Ligands, modified residues, and non-standard cofactors are not supported. Rosetta does not support the CCP4 monomer library, and there is no automatic conversion from CIF files to the **Rosetta format. The most well-tested and easiest to use Rosetta ligand is HEM, for which a CIF file is provided in the Phenix distribution.**
- Alternate conformations are not supported.
- Multi-chain ensembles are not supported.
- Only one model can be refined at a time, and only isotropic refinement at present, for more flexible parameterization you should use phenix.ensemble_refinement.
- Rosetta refinement does not preserve secondary structure, although large structure loss occurs, the performance tends to be worse.
- Rosetta does not support the use of Ramachandran restraints or structures in Rosetta.

Also, the RM for proteins is significantly more processor intensive, although has a faster RM Rosetta (Tiffany et al. 2017) is available, but not yet implemented in the Phenix distribution, and may be in future releases.

Troubleshooting

The program is under development, please address any questions concerning its use to bug@phenix-online.org. The following guidelines may be useful for best performance:

- Rosetta refinement is a stochastic process, and consequently refinement with phenix.rosetta_refine may produce a result that differs from the input model, or which does not improve R-factors or other quality measures. Although the default protocol is designed to be robust for high-resolution and near-native refinement, additional refinement scores will be provided in the future.
- Rosetta refinement is a complex process, and requires a large number of parameters, and may not always give well-behaved refined models and well-behaved R-factors.
- Long runs of Rosetta refinement are not necessarily better than short runs, because Rosetta refinement is a stochastic process, and it may wander away from the starting model if given too many cycles of refinement. If your structure contains weak density or a result of superior optimization, consider using phenix.ensemble_refinement instead.
- Strong Rosetta refinement can produce structures that look ugly or violate the rules of crystallography or stereochemistry, but which have better R-factors than the input model. Rosetta refinement is not in the cell NMR. If the percentage of your molecular replacement solution, we recommend phenix.ensemble_refinement.
- Rosetta refinement is not intended for structures with significant errors in the model, for such cases, consider using phenix.ensemble_refinement instead, such as PDB 2hcb (Terwilliger et al. 2010) with Rosetta.

References

- **Improved low-resolution crystallographic refinement with Phenix and Rosetta.** J. Chiang, R. W. Sheffler, T. C. Terwilliger, P.D. Adams, and T. C. Baker. Nat Methods 9:1265-1268 (2012).
- **Towards automated crystallographic structure refinement with phenix.refine.** P.V. Afonine, R.W. Grosse-Kunstleve, N. Echols, J.J. Headd, N.W. Moriarty, M. Mustyakimov, T.C. Terwilliger, A. Urzhumtsev, P.H. Zwart, and P.D. Adams. Acta Crystallogr. D Biol Crystallogr 68:352-367 (2012).
- **Correcting pervasive errors in RNA crystallography through enumerative structure prediction.** R. Chou, J.J. Gray, P.L. Langan, D. Baker. Nat Methods 7:591-597 (2010). PubMed: 20543838
- **Improved molecular replacement by density- and energy-guided protein structure optimization.** P. Terwilliger, T. Ludtke, R.W. Read, A.J. McCoy, R.D. Oeffner, S.J. Miller, N.W. Grosse-Kunstleve, P.V. Afonine, N.K. Sauter, R.J. Read, D. Baker, P.D. Adams, N. Echols. Acta Crystallogr. D Struct Biol 73:2-11 (2017). PubMed: 28045708
- **Automated structure solution, density modification and model building.** T.C. Terwilliger, R.W. Grosse-Kunstleve, P.V. Afonine, N.W. Moriarty, P.H. Zwart, R.J. Hung, P.D. Adams, N. Echols, T. Alwardt. J Synchrotron Radiat 19:1004-16 (2012). PubMed: 23093766
- **Super-resolution biomolecular crystallography with low-resolution data.** H.F. Schröder, M. Levitt, and D.T. Brunger. Nature 464:1171-4 (2010). PubMed: 20465924

List of all available keywords

Crystallographic refinement, Structure, phenix.1

Python-based Hierarchical Environment for Integrated Crystallography

Running SOLVE/RESOLVE in PHENIX

Author(s)

- Ralf Grosse-Kunstleve, Tom Terwilliger

Purpose

SOLVE and RESOLVE can be run directly in the PHENIX environment. This feature is normally only for advanced SOLVE/RESOLVE users who want to access the keywords in SOLVE/RESOLVE directly.

Usage

Running SOLVE/RESOLVE from the command-line or in a script.

- Write out all data and the keywords.
- Run the command.

This command will set the environmental variables CCP4_OPEN, SOMAP, SOMLIB, and SOLVDIR and call run_solve_resolve.com or run_solve_resolve.csh (if present).

```
phenix.solve -h
```

For a longer version add, chosen / huge, for biggest, / extra, huge.

- Running resolve or resolve pattern in window:

```
phenix.resolve
phenix.resolve pattern
```

- Running solve/resolve from a command file in groups. Here is a command file to run resolve pattern in groups:

```
phenix.resolve
READ pattern.dat
RESOLVE PATTERN FROM 10 TO 50 GROUPS 5 GROUP
TITLE pattern group 5
STOP
```

Literature

Additional information

All the solve/resolve keywords are available in the PHENIX environment of solve and resolve. See the list of keywords and their meanings in the SOLVE/RESOLVE documentation. Documentation is available at http://www.solve.lanl.gov/solve/ , http://www.solve.lanl.gov/ , resolve , and http://www.solve.lanl.gov/ RESOLVE , CCP4 and

Using the PHENIX Wizards

Purpose

Nick Storaski can be run from the PHENIX GUI, from the command line, and from keyboard shortcuts/macros. All three methods can be used to run the same wizard, and all three methods can be used at the same time.

This page describes how to run a Wizard and what a Wizard does in general. The specific Wizard help pages describe the details of each PHENIX Wizard.

Overview of Structure Determination with the PHENIX Wizards

Nick Storaski, Nigel Moriarty, Ralf Grosse-Kunstleve, Paul Adams, Tom Terwilliger, and Peter Zwart. Nick Storaski wrapping our cards and PHENIX. The PHENIX Wizard can also combine SHELXD, MOSFLM, and RESOLVE. Nick Storaski wrapping our cards and PHENIX.

Once you have generated an MR phases, you can use Nick Storaski building blocks, modifications, and refinement with the standard Wizard to improve your model. Finally you can use the Nick Storaski, or Jack Wizard or Tom Wizard to add ligands, water, and ions.

If you generate a phasing model, you can place them using the standard Wizard.

This help page describes how to run the PHENIX Wizard, how to, the command line, or a parameters file. The specific Wizard help pages describe the details of each PHENIX Wizard.

- Automatic Building Wizards using Wizard
- Automatic Building Wizards using Wizard Advanced
- Recombinant Cryo-EM Wizard using LocalCP

Usage

Wizard data directories, sub-directories, facts, and the PDS (Project Data Server)

Wizard can be run from the command line, or used as PHENIX a GUI wizard.

- Wizard can go through with fewer of output files if a subdirectory of your working directory contains the files Wizard needs.
- Wizard can run a Wizard on a remote machine using ssh.
- The subdirectory will keep one or more temporary directories.

Wizard creates intermediate files. These temporary directories will be deleted when the Wizard is finished (unless you set the keep parameter, then, set to TRUE).

If you run Wizard in your PHENIX home, the first GMT image and multiple models will be in a subdirectory of your home directory.

```
~/phenix/1.11-1287/doc/wizard/
```

Wizard can be run from a remote machine and will pop up other information that Wizard generates during its run is stored in the PDS (Project Data Server) directory of the Wizard Pool. The Pool is a set of directories and subdirectories that Wizard uses to keep track of what it has done. Wizard keeps a log of what it has done. Every step is completed by a Wizard. The new Pole are saved (overwriting old ones for that run). In the PDS directory, there is a file called "facts" that contains information about the current Wizard run. Wizard keeps a log of what it has done.

The PDS (Project Data Server) will be in your working directory.

```
./PDS/
```

The PDS contains the output of each of your runs for all Wizards and a record of all the facts (parameters and values) that Wizard has used. Wizard keeps a log of what it has done. Wizard keeps a log of what it has done. Wizard stores "facts" in the corresponding entries in the PDS and also defined. You can copy the PDS from one place to another and Wizard will continue where it left off. Wizard keeps a log of what it has done. Wizard keeps a log of what it has done. Wizard keeps a log of what it has done. Wizard keeps a log of what it has done.

Running a Wizard using a multicomputer machine or a cluster

Wizard can be run on a multicomputer machine or a cluster. Wizard can be run on a multicomputer machine or a cluster. Wizard can be run on a multicomputer machine or a cluster. Wizard can be run on a multicomputer machine or a cluster. Wizard can be run on a multicomputer machine or a cluster.

Usage

```
phenix.wizard
```

to command line command for a Wizard will use a programme to run the wizard (if possible). Normally you will run the wizard processes in the background and the output of

```
phenix.wizard > wizard.log &
```

If you have a cluster with a batch queue, you can send subprocesses to the batch queue with

```
-c,--queuecmd
```

(or whatever your batch command is). In this case you will use

```
-q,--queue
```

so that the batch queue can make best of your jobs.

The Wizards divide the data into stretch batches during processing. The value of

```
-bsize=100
```

is set from 1 to the default (depending on the Wizard) and is appropriate if you have up to stretch processors. If you have more than 100 processors, you should set bsize to the number of processors. If you have more than 100 processors, you should set bsize to the number of processors. If you have more than 100 processors, you should set bsize to the number of processors. If you have more than 100 processors, you should set bsize to the number of processors.

Running a Wizard from a GUI

Basic operation of a Wizard from the GUI

- Start up the PHENIX GUI in your working directory by typing "phenix".
- Wizard will ask you for the Wizard you want to run. Wizard will ask you for the Wizard ("Autofit") under Wizards. Wizard will ask you for the Wizard (Wizard) under Wizards.
- Wizard will ask you for the Wizard (Wizard) under Wizards. Wizard will ask you for the Wizard (Wizard) under Wizards.
- The Wizard will come up in a new window and will open a grey Parameterizer window asking you for parameters. Wizard will ask you for parameters.
- Enter the Wizard and the data directory (or accept the default). Wizard will ask for the data directory. Wizard will ask for the data directory. Wizard will ask for the data directory. Wizard will ask for the data directory.
- Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters.
- Wizard is the next window by pitching "Continue" in the upper left corner of the grey Parameters window. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters.
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Keeping track of multiple runs of a Wizard from the GUI

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Setting parameters of a Wizard from the GUI

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Running a Wizard from the command-line

Basic operation of a Wizard from the command-line

- You can run a wizard from the command line by the command in the Wizard's manual.

```
phenix.wizard phenix.xyz log.refinedpdb -k 1 -b
```

- Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters.
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Keeping track of multiple runs of a Wizard from the command-line

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Setting parameters of a Wizard from the command-line

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Running a Wizard from the command-line

Basic operation of a Wizard from the command-line

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Keeping track of multiple runs of a Wizard from the command-line

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Setting parameters of a Wizard from the command-line

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Running a Wizard from a parameters file

Parameters files are an easy way to specify any parameters that you want to use when running a Wizard. They are also useful when you want to run a Wizard with a set of parameters that you have used before.

You can put a parameters file in with what you would by running the wizard with the flag "-ofmt phenix".

```
phenix.wizard -ofmt phenix
```

Wizard will write a file called "wizard.eff" (or a GIS dialogue with "phenix.wizard.eff").

```
wizard {
  data = "./data/*.mtz"
  seq_file = "./sequence.dat"
  ncycle = 3
  nsite = 10
  resolution = 2.0 or 0.05 NA 20.0 NA 2.0
  ncycle = 3
  nsite = 10
  resolution = 2.0
  ncycle = 3
  nsite = 10
  resolution = 2.0
}
```

Note that one keyword ("data=wizard" in "wizard.eff") followed by quoted brackets ({ ... }) which encloses sets of parameters for the Wizard.

The values of parameters are usually entered on one line, without quotation marks (as in the example) unless they are to be of uncertainties as a single field.

Wizard will accept and ignoring either a parameters file or on the command line. In the above example you could Wizard with

```
phenix.wizard data="./data/*.mtz" seq_file="./sequence.dat"
```

or

```
phenix.wizard wizard.eff
```

At the end of every Wizard run, Wizard writes the output in two details.

```
wizard.eff
```

- NOTE that you can set one SGUIDE, BSGUIDE or MSGUIDE, PATTERN keyword in PHENIX using the "phenix.wizard.guide" command. Wizard will use the guide to determine the parameters to use in the Wizard. The Wizard is a Wizard, so you have to run two steps of guide around the command line first:

```
phenix.wizard -ofmt phenix.wizard.guide -- -ofmt -- -ofmt phenix
```

- Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters. Wizard will ask you for parameters.
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Specific limitations and problems:

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Literature

Additional information

Phenix (PHENIX Automated Molecular Refinement for Enzymatic Kinetics)

Download the data from PDB and setting up for SAD structure determination with phenix.sad_data_from_pdb

Author(s)

- phenix.sad_data_from_pdb: Tom Terwilliger

Purpose

phenix.sad_data_from_pdb is a command line tool for downloading coordinates and anomalous structure factor data from the PDB, preparing it and setting up for running SAD or MAD experiments of data on ISRP datasets.

Usage

How phenix.sad_data_from_pdb works:

phenix.sad_data_from_pdb first uses phenix.fetch_pdb to download the data from the PDB.

Then it converts the structure factor data to Scalepack unmerged original data format, calculates model map coefficients, and finds the sites of the anomalous scatterers. It then uses phenix.ISRP to find the best data and set the resolution of the data. If there are not phases in the PDB deposition then the processed data will not work.

Examples

Standard run of phenix.sad_data_from_pdb:

Running phenix.sad_data_from_pdb simply: You can just type:

```
phenix.sad_data_from_pdb
```

and phenix.sad_data_from_pdb will download the data for 1ubd and set up a directory with the data and with the appropriate parameters for phenix.ISRP and phenix.autosol. If phenix.ISRP finds a good dataset, phenix.autosol will run, solution will be found that is suitable for running phenix.autosol using that anomalous data.

Possible Problems

Specific limitations and problems:

Literature

Additional information:

List of all available keywords

data_directory = None	Directory where files are to be located
pdb_id = None	PDB ID to fetch pdb and ds or ISRP SAD dataset
ds_file = None	Name of ds file (default is pdb_id.ds in current directory)
ha_file = None	File of anomalous scattering atom type (atom_type.sca) and scattered f' and f'' (default is ha.sca)
chain = PROTEIN NUCLEIC_ACID	Which chain(s) to use. Default is all protein and nucleic acid chains. Enter PROTEIN or NUCLEIC_ACID to use all protein or all nucleic acid chains, or enter chain ID(s) (e.g. A,B) to use specified chains.
	Note: if 1ubd is used, 1ubd downloaded files have the PDB ID 1ZLD.
	Note: if 1ubd is used, the ISRP dataset is not found by ISRP but the corresponding dataset is found if the resolution is specified.
	Note: if 1ubd is used, the ISRP dataset is found by ISRP but the resolution is not correct unless the resolution is specified.
	Note: the default resolution for 1ubd is 1.5 Angstroms.
anomalous = None	Use anomalous scattering data in the PDB structure
keep_pdb = True	Keep PDB and other intermediate scattering and ignore that already exists
verbose = True	Verbose output
cleanup_temp_files = None	Do not change the temp directory name for a single session

scale_and_merge

Scaling unmerged anonymous data or multiple datasets with scale_and_merge

Author(s)

* Lara Jehl, Holger Rarbi, Tom Weiergräber

Purpose

scale_and_merge is a tool for scaling unmerged anonymous data or multiple data files and creating a joint merged and free scaled MTZ file. The tool normally is used in combination with aimless, pointless or cross-validation and ensures consistent scaling of the data between all files and can be used in cross-validation analysis.

Usage

How scale_and_merge works:

* The program scale_and_merge uses a reference containing datasets in the name of a large unmerged MTZ file.
* The program splits the reference into individual datasets and runs aimless on each dataset to obtain the standard error adjustment factors and to get a good estimate with cleaned reads partially over-scaled. Each refined dataset is then merged and the standard error adjustment factors are applied to the unmerged data.
* scale_and_merge will then check the set of intensities of all the datasets. Normally it will change the merged data to unmerged intensities and run aimless on the unmerged data to obtain a scaled MTZ file. Alternatively, if specified, the intensities will be written into unmerged intensities to be scaled by aimless.
* The program then calculates the correlation between the intensities of each dataset and the merged data and identifies outliers. Outliers are identified by a user-defined threshold of the Pearson's correlation coefficient. Alternatively, a user-specified set of datasets can be used for the scaling and merging of the data. The information is saved in a file and can be used for cross-validation analysis of the data or for manual scaling.
* The program then calculates the standard error adjustment factors for the final scaling, combining them in the intensity statistics with Aimless writing to scaled.log and mtzdump from all SigmaFac.
* The program then calculates the standard error adjustment factors for the final scaling and combines them in the intensity statistics with Aimless writing to scaled.log and mtzdump from all SigmaFac.
* In the final scaling the individual datasets are cross scaled with simple rotation and a B-factor for each dataset. Alternatively, the user can specify a set of datasets to be used for the final scaling. The calculation of systematic differences between datasets and the mean are calculated based on the log-transformed intensities and the differences are written into a file. Alternatively, the user can specify a set of datasets to be used for the scaling and the final scaling is then performed. The program changes the standard error adjustment factors for the final scaling to the values from the last run of aimless.
* A generalized differences approach is applied with optimize.py/optimize.Pruning, changing a normal set of differences into a set of differences that minimizes the differences between the data and the mean. The output indicates if the differences set of data reduces the mean or not more or less. The data is calculated with the original data and the differences set of data. The program then calculates the standard error of the intensity differences from the merged dataset to optimize individual standard error adjustment factors. The program then calculates the standard error adjustment factors for the final scaling and combines them in the intensity statistics with Aimless writing to scaled.log. Finally, the program calculates the final merged data with the optimized standard error adjustment factors and the optimized differences set of data. The output is written into a file. The program then calculates the standard error adjustment factors for the final scaling and combines them in the intensity statistics with Aimless writing to scaled.log. The output files.
* The program then calculates the final scale factors for the output of two half-sets. These half-sets are used for estimating the quality of the data and are used in anomalous signal for this analysis.
* The program then calculates the final scale factors for the output of two half-sets. These half-sets are used for estimating the quality of the data and are used in anomalous signal for this analysis. The program calculates the standard error adjustment factors for the final scaling and combines them in the intensity statistics with Aimless writing to scaled.log. The output files are written to a file. The program calculates the standard error adjustment factors for the final scaling and combines them in the intensity statistics with Aimless writing to scaled.log. The output files are written to a file. The first half-set dataset is one half dataset and the second half is the other. The third preferred dataset is the merged dataset. The program calculates the standard error adjustment factors for the final scaling and combines them in the intensity statistics with Aimless writing to scaled.log. The output files are written to a file. The program calculates the standard error adjustment factors for the final scaling and combines them in the intensity statistics with Aimless writing to scaled.log. These datasets are used for estimating the quality of the data and are used in anomalous signal for this analysis.
* The program then calculates the final scale factors for the output of two half-sets. These half-sets are used for estimating the quality of the data and are used in anomalous signal for this analysis.
* Optional: If the unmerged and observed, the correlation of anomalous differences between half datasets is calculated.

Output from scale_and_merge

scale_and_merge provides a summary half dataset correlations in your dataset. Here is an example with very low anomalous signal (but useless):

```
scale_and_merge -f /path/to/reference -d DATA DATA
Using reference:
/path/to/reference
Using data:
/path/to/data_1/DATA
/path/to/data_2/DATA
Using:
/usr/local/bin/aimless
/usr/local/bin/mtzdump
/usr/local/bin/cmtzcad
/usr/local/bin/cmtzsort
/usr/local/bin/cmtzmerge
/usr/local/bin/cmtzsplit
/usr/local/bin/cmtzrsf
/usr/local/bin/cmtzsf
/usr/local/bin/cmtzsigfac
/usr/local/bin/cmtzsigfac
/usr/local/bin/cmtzsigfac
```

```
start_time
  date : Date
```

Indicates date and time of a run date in ISO 8601 extended format or time in UTC in ISO 8601 extended format. Used in conjunction with the start_time_fractional field to define a fractional second. Example: "2011-12-13T04:51:03" for a run starting exactly on December 13th 2011 at 4:51:03 AM UTC. Example: "04:51:03" for a run starting exactly at 4:51:03 AM UTC on an unspecified date.

```
  time_zone_abbreviation_name : Text
```

Abbreviation or identifier for the time zone in which the start_time is specified. Example: "EST" for Eastern Standard Time in the United States. Example: "Europe/London" for the time zone used in London, United Kingdom. Note that the start_time field is in UTC, so this field is only used to indicate the time zone in which the start_time was originally specified. Note that the start_time field is in UTC because it is difficult to specify a fractional second in a local time zone because of daylight savings time.

```
  start_time_fractional : Real
```

The fractional part of the start_time. Used in conjunction with the start_time field to define a fractional second. Example: 0.123 for a run starting at 123 milliseconds after the start_time.

```
  start_time_date_index : Date
```

Indicates date and time of a run date in ISO 8601 extended format or time in UTC in ISO 8601 extended format. Used in conjunction with the start_time_fractional field to define a fractional second. Example: "2011-12-13T04:51:03" for a run starting exactly on December 13th 2011 at 4:51:03 AM UTC. Example: "04:51:03" for a run starting exactly at 4:51:03 AM UTC on an unspecified date.

```
  start_time_fractional_index : Real
```

The fractional part of the start_time. Used in conjunction with the start_time_date_index field to define a fractional second. Example: 0.123 for a run starting at 123 milliseconds after the start_time.

```
  start_time_index : Date-Time
```

Indicates date and time of a run date in ISO 8601 extended format or time in UTC in ISO 8601 extended format. Used in conjunction with the start_time_fractional field to define a fractional second. Example: "2011-12-13T04:51:03" for a run starting exactly on December 13th 2011 at 4:51:03 AM UTC. Example: "04:51:03" for a run starting exactly at 4:51:03 AM UTC on an unspecified date.

```
  start_time_fractional_index : Real
```

The fractional part of the start_time. Used in conjunction with the start_time_index field to define a fractional second. Example: 0.123 for a run starting at 123 milliseconds after the start_time.

```
  run_type : Text
```

Indicates the type of run. Example: "Test" for a test run, "Production" for a production run.

```
  run_identifier : Text
```

Indicates the identifier for the run. Example: "Run 1" for a run with the identifier "Run 1".

```
  run_description : Text
```

Indicates the description for the run. Example: "Run 1 was a test run to verify the new sensor was working properly." for a run with the description "Run 1 was a test run to verify the new sensor was working properly."

```
  run_operator_name : Text
```

Indicates the name of the operator who performed the run. Example: "Jane Smith" for a run performed by Jane Smith.

```
  run_operator_id : Text
```

Indicates the identifier for the operator who performed the run. Example: "1234" for a run performed by the operator with the identifier "1234".

```
  run_operator_email : Text
```

Indicates the email address for the operator who performed the run. Example: "jsmith@example.com" for a run performed by the operator with the email address "jsmith@example.com".

```
  run_operator_phone_number : Text
```

Indicates the phone number for the operator who performed the run. Example: "+1-555-123-4567" for a run performed by the operator with the phone number "+1-555-123-4567".

```
  run_operator_organization : Text
```

Indicates the organization for the operator who performed the run. Example: "Acme Corporation" for a run performed by the operator with the organization "Acme Corporation".

```
  run_operator_organization_id : Text
```

Indicates the identifier for the organization for the operator who performed the run. Example: "1234" for a run performed by the operator with the organization identifier "1234".

```
  sensor
    sensor_serial_number : Text
```

Indicates the serial number of the sensor. Example: "SN-12345" for a sensor with the serial number "SN-12345".

```
    sensor_model_number : Text
```

Indicates the model number of the sensor. Example: "MN-12345" for a sensor with the model number "MN-12345".

```
    sensor_firmware_version : Text
```

Indicates the firmware version of the sensor. Example: "v1.2.3" for a sensor with the firmware version "v1.2.3".

```
    sensor_hardware_version : Text
```

Indicates the hardware version of the sensor. Example: "v1.2.3" for a sensor with the hardware version "v1.2.3".

```
    sensor_manufacturer : Text
```

Indicates the manufacturer of the sensor. Example: "Acme Corporation" for a sensor manufactured by Acme Corporation.

```
    sensor_manufacturer_id : Text
```

Indicates the identifier for the manufacturer of the sensor. Example: "1234" for a sensor manufactured by the manufacturer with the identifier "1234".

```
    sensor_manufacturer_organization_name : Text
```

Indicates the name of the organization that manufactured the sensor. Example: "Acme Corporation" for a sensor manufactured by Acme Corporation.

```
    sensor_manufacturer_organization_id : Text
```

Indicates the identifier for the organization that manufactured the sensor. Example: "1234" for a sensor manufactured by the organization with the identifier "1234".

```
  crystal_info
    crystal_type : Text
```

Indicates the type of crystal used in the data file. Example: "Quartz" for a data file created using a quartz crystal.

```
    has_calibration : Boolean
```

Indicates whether the data file has been calibrated. Example: "true" for a data file that has been calibrated.

```
    data_quality : Text
```

Indicates the quality of the data file. Example: "Good" for a data file that is of good quality.

```
  data_collection
    sensor_data_file_type : Text
```

Indicates the type of sensor data file. Example: "Raw" for a data file that contains raw sensor data.

```
    sensor_data_file_format : Text
```

Indicates the format of the sensor data file. Example: "CSV" for a data file that is in the CSV format.

```
    raw_data_file : Text
```

Indicates the name of the raw data file. Example: "raw_data.csv" for a data file that is named "raw_data.csv".

```
    data_collection_datapoint : Text
```

Indicates the name of the datapoint in the data file that contains the data collection datapoint. Example: "data_collection" for a data file that contains the data collection datapoint.

```
    data_collection_header_datapoint : Text
```

Indicates the name of the datapoint in the data file that contains the data collection header datapoint. Example: "data_collection_header" for a data file that contains the data collection header datapoint.

```
    data_collection_header_datapoint_index : Real
```

Indicates the index of the datapoint in the data file that contains the data collection header datapoint. Example: "1" for a data file that contains the data collection header datapoint at index 1.

```
    sensor_data_header_datapoint : Text
```

Indicates the name of the datapoint in the data file that contains the sensor data header datapoint. Example: "sensor_data_header" for a data file that contains the sensor data header datapoint.

```
    sensor_data_header_datapoint_index : Real
```

Indicates the index of the datapoint in the data file that contains the sensor data header datapoint. Example: "2" for a data file that contains the sensor data header datapoint at index 2.

```
    sensor_data_header_datapoint_offset : Real
```

Indicates the offset in the data file that contains the sensor data header datapoint. Example: "0" for a data file that contains the sensor data header datapoint at offset 0.

```
    sensor_data_header_datapoint_length : Real
```

Indicates the length of the sensor data header datapoint in the data file. Example: "100" for a data file that contains the sensor data header datapoint of length 100.

```
    sensor_data_header_datapoint_checksum : Text
```

Indicates the checksum of the sensor data header datapoint in the data file. Example: "1234" for a data file that contains the sensor data header datapoint with checksum "1234".

```
    sensor_data_header_datapoint_checksum_type : Text
```

Indicates the type of checksum used for the sensor data header datapoint in the data file. Example: "CRC-32" for a data file that contains the sensor data header datapoint with checksum type "CRC-32".

```
    sensor_data_header_datapoint_checksum_byte_order : Text
```

Indicates the byte order used for the checksum of the sensor data header datapoint in the data file. Example: "Little Endian" for a data file that contains the sensor data header datapoint with checksum byte order "Little Endian".

```
    sensor_data_header_datapoint_checksum_offset : Real
```

Indicates the offset of the checksum of the sensor data header datapoint in the data file. Example: "100" for a data file that contains the sensor data header datapoint with checksum offset 100.

```
    sensor_data_header_datapoint_checksum_length : Real
```

Indicates the length of the checksum of the sensor data header datapoint in the data file. Example: "4" for a data file that contains the sensor data header datapoint with checksum length 4.

```
  sensor
    sensor_serial_number : Text
```

Indicates the serial number of the sensor. Example: "SN-12345" for a sensor with the serial number "SN-12345".

```
    sensor_model_number : Text
```

Indicates the model number of the sensor. Example: "MN-12345" for a sensor with the model number "MN-12345".

```
    sensor_firmware_version : Text
```

Indicates the firmware version of the sensor. Example: "v1.2.3" for a sensor with the firmware version "v1.2.3".

```
    sensor_hardware_version : Text
```

Indicates the hardware version of the sensor. Example: "v1.2.3" for a sensor with the hardware version "v1.2.3".

```
    sensor_manufacturer : Text
```

Indicates the manufacturer of the sensor. Example: "Acme Corporation" for a sensor manufactured by Acme Corporation.

```
    sensor_manufacturer_id : Text
```

Indicates the identifier for the manufacturer of the sensor. Example: "1234" for a sensor manufactured by the manufacturer with the identifier "1234".

```
    sensor_manufacturer_organization_name : Text
```

Indicates the name of the organization that manufactured the sensor. Example: "Acme Corporation" for a sensor manufactured by Acme Corporation.

```
    sensor_manufacturer_organization_id : Text
```

Indicates the identifier for the organization that manufactured the sensor. Example: "1234" for a sensor manufactured by the organization with the identifier "1234".

```
  sensor_data
    sensor_data_header_version : Text
```

Indicates the version of the sensor data header. Example: "v1.2.3" for a sensor data header with version "v1.2.3".

```
    sensor_data_header_length : Real
```

Indicates the length of the sensor data header. Example: "100" for a sensor data header of length 100.

```
    sensor_data_header_checksum : Text
```

Indicates the checksum of the sensor data header. Example: "1234" for a sensor data header with checksum "1234".

```
    sensor_data_header_checksum_type : Text
```

Indicates the type of checksum used for the sensor data header. Example: "CRC-32" for a sensor data header with checksum type "CRC-32".

```
    sensor_data_header_checksum_byte_order : Text
```

Indicates the byte order used for the checksum of the sensor data header. Example: "Little Endian" for a sensor data header with checksum byte order "Little Endian".

```
    sensor_data_header_checksum_offset : Real
```

Indicates the offset of the checksum of the sensor data header. Example: "100" for a sensor data header with checksum offset 100.

```
    sensor_data_header_checksum_length : Real
```

Indicates the length of the checksum of the sensor data header. Example: "4" for a sensor data header with checksum length 4.

```
    sensor_data_header_data : Text
```

Indicates the sensor data header. Example: "0x1234" for a sensor data header with the hexadecimal value "0x1234".

```
    sensor_data_header_data_encoding : Text
```

Indicates the encoding used for the sensor data header. Example: "Base64" for a sensor data header encoded in Base64.

```
    sensor_data_header_data_encoding_type : Text
```

Indicates the type of encoding used for the sensor data header. Example: "Hexadecimal" for a sensor data header encoded in hexadecimal.

```
    sensor_data_header_data_encoding_length : Real
```

Indicates the length of the encoding used for the sensor data header. Example: "100" for a sensor data header encoded in Base64 of length 100.

```
    sensor_data_header_data_encoding_checksum : Text
```

Indicates the checksum of the encoding used for the sensor data header. Example: "1234" for a sensor data header encoded in Base64 with checksum "1234".

```
    sensor_data_header_data_encoding_checksum_type : Text
```

Indicates the type of checksum used for the encoding used for the sensor data header. Example: "CRC-32" for a sensor data header encoded in Base64 with checksum type "CRC-32".

```
    sensor_data_header_data_encoding_checksum_byte_order : Text
```

Indicates the byte order used for the checksum of the encoding used for the sensor data header. Example: "Little Endian" for a sensor data header encoded in Base64 with checksum byte order "Little Endian".

```
    sensor_data_header_data_encoding_checksum_offset : Real
```

Indicates the offset of the checksum of the encoding used for the sensor data header. Example: "100" for a sensor data header encoded in Base64 with checksum offset 100.

```
    sensor_data_header_data_encoding_checksum_length : Real
```

Indicates the length of the checksum of the encoding used for the sensor data header. Example: "4" for a sensor data header encoded in Base64 with checksum length 4.

```
    sensor_data_header_data_encoding_checksum_data : Text
```

Indicates the checksum data of the encoding used for the sensor data header. Example: "0x1234" for a sensor data header encoded in Base64 with checksum data "0x1234".

```
    sensor_data_header_data_encoding_checksum_data_encoding : Text
```

Indicates the encoding used for the checksum data of the encoding used for the sensor data header. Example: "Hexadecimal" for a sensor data header encoded in Base64 with checksum data encoded in hexadecimal.

```
    sensor_data_header_data_encoding_checksum_data_encoding_type : Text
```

Indicates the type of encoding used for the checksum data of the encoding used for the sensor data header. Example: "Hexadecimal" for a sensor data header encoded in Base64 with checksum data encoded in hexadecimal.

```
    sensor_data_header_data_encoding_checksum_data_encoding_length : Real
```

Indicates the length of the encoding used for the checksum data of the encoding used for the sensor data header. Example: "100" for a sensor data header encoded in Base64 with checksum data encoded in hexadecimal of length 100.

```
  sensor
    sensor_serial_number : Text
```

Indicates the serial number of the sensor. Example: "SN-12345" for a sensor with the serial number "SN-12345".

```
    sensor_model_number : Text
```

Indicates the model number of the sensor. Example: "MN-12345" for a sensor with the model number "MN-12345".

```
    sensor_firmware_version : Text
```

Indicates the firmware version of the sensor. Example: "v1.2.3" for a sensor with the firmware version "v1.2.3".

```
    sensor_hardware_version : Text
```

Indicates the hardware version of the sensor. Example: "v1.2.3" for a sensor with the hardware version "v1.2.3".

```
    sensor_manufacturer : Text
```

Indicates the manufacturer of the sensor. Example: "Acme Corporation" for a sensor manufactured by Acme Corporation.

```
    sensor_manufacturer_id : Text
```

Indicates the identifier for the manufacturer of the sensor. Example: "1234" for a sensor manufactured by the manufacturer with the identifier "1234".

```
    sensor_manufacturer_organization_name : Text
```

Indicates the name of the organization that manufactured the sensor. Example: "Acme Corporation" for a sensor manufactured by Acme Corporation.

```
    sensor_manufacturer_organization_id : Text
```

Indicates the identifier for the organization that manufactured the sensor. Example: "1234" for a sensor manufactured by the organization with the identifier "1234".

```
  sensor_data
    sensor_data_header_version : Text
```

Indicates the version of the sensor data header. Example: "v1.2.3" for a sensor data header with version "v1.2.3".

```
    sensor_data_header_length : Real
```

Indicates the length of the sensor data header. Example: "100" for a sensor data header of length 100.

```
    sensor_data_header_checksum : Text
```

Indicates the checksum of the sensor data header. Example: "1234" for a sensor data header with checksum "1234".

```
    sensor_data_header_checksum_type : Text
```

Indicates the type of checksum used for the sensor data header. Example: "CRC-32" for a sensor data header with checksum type "CRC-32".

```
    sensor_data_header_checksum_byte_order : Text
```

Indicates the byte order used for the checksum of the sensor data header. Example: "Little Endian" for a sensor data header with checksum byte order "Little Endian".

```
    sensor_data_header_checksum_offset : Real
```

Indicates the offset of the checksum of the sensor data header. Example: "100" for a sensor data header with checksum offset 100.

```
    sensor_data_header_checksum_length : Real
```

Indicates the length of the checksum of the sensor data header. Example: "4" for a sensor data header with checksum length 4.

```
    sensor_data_header_data : Text
```

Indicates the sensor data header. Example: "0x1234" for a sensor data header with the hexadecimal value "0x1234".

```
    sensor_data_header_data_encoding : Text
```

Indicates the encoding used for the sensor data header. Example: "Base64" for a sensor data header encoded in Base64.

```
    sensor_data_header_data_encoding_type : Text
```

Indicates the type of encoding used for the sensor data header. Example: "Hexadecimal" for a sensor data header encoded in hexadecimal.

```
    sensor_data_header_data_encoding_length : Real
```

Indicates the length of the encoding used for the sensor data header. Example: "100" for a sensor data header encoded in Base64 of length 100.

```
    sensor_data_header_data_encoding_checksum : Text
```

Indicates the checksum of the encoding used for the sensor data header. Example: "1234" for a sensor data header encoded in Base64 with checksum "1234".

```
    sensor_data_header_data_encoding_checksum_type : Text
```

Indicates the type of checksum used for the encoding used for the sensor data header. Example: "CRC-32" for a sensor data header encoded in Base64 with checksum type "CRC-32".

```
    sensor_data_header_data_encoding_checksum_byte_order : Text
```

Indicates the byte order used for the checksum of the encoding used for the sensor data header. Example: "Little Endian" for a sensor data header encoded in Base64 with checksum byte order "Little Endian".

```
    sensor_data_header_data_encoding_checksum_offset : Real
```

Indicates the offset of the checksum of the encoding used for the sensor data header. Example: "100" for a sensor data header encoded in Base64 with checksum offset 100.

```
    sensor_data_header_data_encoding_checksum_length : Real
```

Indicates the length of the checksum of the encoding used for the sensor data header. Example: "4" for a sensor data header encoded in Base64 with checksum length 4.

```
    sensor_data_header_data_encoding_checksum_data : Text
```

Indicates the checksum data of the encoding used for the sensor data header. Example: "0x1234" for a sensor data header encoded in Base64 with checksum data "0x1234".

```
    sensor_data_header_data_encoding_checksum_data_encoding : Text
```

Indicates the encoding used for the checksum data of the encoding used for the sensor data header. Example: "Hexadecimal" for a sensor data header encoded in Base64 with checksum data encoded in hexadecimal.

```
    sensor_data_header_data_encoding_checksum_data_encoding_type : Text
```

Indicates the type of encoding used for the checksum data of the encoding used for the sensor data header. Example: "Hexadecimal" for a sensor data header encoded in Base64 with checksum data encoded in hexadecimal.

```
    sensor_data_header_data_encoding_checksum_data_encoding_length : Real
```

Indicates the length of the encoding used for the checksum data of the encoding used for the sensor data header. Example: "100" for a sensor data header encoded in Base64 with checksum data encoded in hexadecimal of length 100.

Phenix *Python based Hierarchical Environment for Integrated Crystallography*

Simplified Carbohydrate Line-Entry System (SCALES)

There are many formats for specifying a carbohydrate to enter in the chemical field. Hough et al. (1976

The article introduces a formal known as WLNOTT.

A common and compact molecule specification format is known as SMILES (left) which stands for: SI nodes on the Line Notation for Chemical Structures and Reactions. Its successor is SMARTS (Arthur Weininger 1988) which also has atoms.

Without stereochemistry, the only delimiters are parentheses and numbers. Atoms are specified by their symbols. Bonds are implicit (only the one-letter elements are allowed) and assumed to be single unless specified otherwise. Rings are denoted by an arbitrary number and are connected by matching numbers. Branches are denoted by parentheses. Stereochemistry is specified using slashes and backslashes. Rings are denoted by matching numbers. There are more rules for this, complicating the specification. Although the notation is compact, it is difficult to read and write for carbohydrates, which are carbohydrates. (L.G.)

Carbohydrates are typically linked one of two ways: one linking to the end of the polysaccharide. For instance, the α-glucose that constitutes the polymer, for the most common glycosidic attachment is written 1-4 or 1-α-4. The 1 specifies the carbon on the first sugar, the α specifies the stereochemistry of the bond, and the 4 is written in SMILES, WLNOTT, PDB. (L.G.) It is not a step to imagine that this could be represented using SMARTS. (L.G.)

- 2010-06-09:

The PDB Chemical Component Dictionary is a simple text file in PDB format. The ATOM and HETATM records are identical to the PDB format. The CONECT records are different. The CONECT records specify the connectivity of the atoms. The bond order is specified using the bond order specifier. The bond order specifier is a single character. The bond order specifier is the character immediately after the atom serial number. The bond order specifier is optional. If the bond order specifier is not present, the bond order is assumed to be a single bond.

- 2011-06-09:

The PDB Chemical Component Dictionary is a simple text file in PDB format. The ATOM and HETATM records are identical to the PDB format. The CONECT records are different. The CONECT records specify the connectivity of the atoms. The bond order specifier is a single character. The bond order specifier is the character immediately after the atom serial number. The bond order specifier is optional. If the bond order specifier is not present, the bond order is assumed to be a single bond.

words

Phenix

Action-Issue Hierarchical Environment for Integrated Bibliography

phenix.scedc: SCEDS - identify domains with normal mode analysis

Description

SCEDS is useful for identifying domains in a cluster to be used by molecular replacement where it is anticipated that the domain movements between the two states will be dominated by the lowest frequency normal mode vibrations. Typically it is in cases that correspondence up to a low resolution is found using domains derived from the target structure, but the correct solution is not found because the domains have moved too far from their positions in the adjacent homolog and solution. A deeper analysis then would otherwise have been possible. Domains are identified using a cluster analysis of the lowest frequency normal modes.

To use SCEDS supply it with the PDB model and execute it. Depending on the size of the model it may take some time to run. Output is written to the screen.

Output is one or more domains each saved into separate pdb files. These can then be used in molecular replacement. It is good practice to inspect the identified domains in a graphical viewer such as chimera or Pymol.

Chimera - Chimera
Chimera
Chimera

List of all available keywords

```
file_name : "test"
file_ext : "dat"
mp_prefix_ok : false
mp_prefix : "mp"
delimiter : " "                                  Use tilde as PRAGMA SEQ, not used if command line
delimiter_escape : false
keywords
    ebm
        kind : 1
        continuous : 0
    eye
        resolution : 1024.0[]
        fix_duration : 0.0[]
        fix_precision : 0.0
        fix_x : 0.0
        fix_y : 0.0
        focus : 0
    person
        id : "unknown" (<20 B)
        ml : false
        ms
            item : 0
            duration : 0.0
            duration_ms : 0.0 (rounded duration) (ms)
    scene
        width : 0 (mm)
        kind : 0
        weight
            weight : 0.0
            weight_x : 0.0
            weight_y : 0.0
            weight_z : 0.0
    ebc
        item : 0
        kind : "Blue Circle Test"
        distance
            distance : 0.0
            mm : 0.0
            px : 0.0
        resolution
            mm : 0.0
            px : 0.0
        resolution
            mm : 0.0
            px : 0.0
        size
            mm : 0.0
            px : 0.0
```

Model preparation with wsdpf_ensemble

Contents
- Purpose
- Usage
  - Input files
  - Output files
- Description
- Output files
- Compatibility
  - Other EMBOSS applications
  - EDAM ontology
  - Input and output formats
    - List of available keywords

Purpose

wsdpf_ensemble is a certified model preparation program that internally uses modeller and freesasa. While these two programs are not separately distributed in EMBOSS, wsdpf_ensemble provides a simple interface to the underlying functionality. The output of wsdpf_ensemble is suitable for other EMBOSS programs to information how solvent and there are further benefits as well.

Usage

The program wsdpf_ensemble is available from the command line and will also be available from the EMBOSS GUI.

Input files

Input Sequence: Multiple(s) sequence(s) to be superimposed and modelled. For each sequence, specify gene name as the external using MASSA alignment options, and separately information can be associated with the sequence. Sequence can be read from standard input, or from a file specified by the -sequence qualifier.

Input sequence (sequence)

Acceptable formats: FASTA, Nonspecific sequences, gcg, ncbi

- **Sequence Files**: target sequences (for each sequence position). This is used to identify the target sequence, and to provide information about the sequence. Sequence files are optional, but if they are specified, sequence quality is available. -scale scales sequence qualityscale scale factor applied to the sequence quality. -sfmt specifies the sequence file format. Acceptable formats are: -sfmt FASTA fasta, -sfmt PIR PIR/NBRF, -sfmt PIR PIR/NBRF and -sfmt GCG GCG/MSF, -sfmt EMBLDAT EMBL/EMBLNEW, -sfmt SWISS SwissProt, -sfmt PDB PDB/ENT and -sfmt ALN ALN/CLUSTALW.
- **Alignments**: sequence alignment with the target sequence. The alignment contains information that can be used to identify the target sequence, and to provide information about the sequence. Alignments are automatically associated with the corresponding alignment based on a sequence comparison. The target sequence is automatically added to the alignment if it is not present. Alignments are optional, and if they are omitted the sequence is long alignment is read as target. Alignment is optional. -scale scale factor applied to the alignment quality. -afmt specifies the alignment file format. Acceptable formats are: -afmt CLUSTALW ALN, -afmt FASTA fasta, -afmt PIR PIR/NBRF and -afmt EMBLDAT EMB Stockholm.
- **Sequence Quality**: Sequence quality is used to weight the sequence in the alignment and to weight the sequence when the sequence is long alignment is read as target. Sequence quality is optional. -scale scale factor applied to the sequence quality. -qfmt specifies the quality file format. Acceptable formats are: -qfmt GCG GCG/MSF, -qfmt PIR PIR/NBRF, -qfmt EMBLDAT EMBL/EMBLNEW and -qfmt SWISS SwissProt.

Output files

Output Sequence: Output sequence(s) (sequence). The file is written according to the following conventions: -out sequence outfile where -out is a new method parameter. (accepted from the -outseq option), and is similar to -seqout output data type. (-outseq)

Description

The program loads in the input files, creates assembly, and runs assemblies from the assemblies.txt file. The assemblies.txt file contains a list of assemblies to be processed, one per line. Each assembly is processed in the order specified in the assemblies.txt file. Assembly names must match the assembly definitions in the assembly-definitions folder. Assembly definitions are JSON files that specify the input files, output file, and optional transformations to apply to the data.

In case there is only a single assembly present, the assemblies.txt step is skipped, and the program starts at the assembly specified in the assembly-definitions folder processing the input files in order, in which case the program accepts any assembly name.

Trimming

Gene.prank also supports trimming from Clustalw, but unlike the aln2fa option in Translatorx, this is available as the default option. Trimming is controlled by the -trimfactor option in translatorx. In addition, this can also be used in combination with pairwise options.

Command line

```
Gene.prank [options]
-d=[name]   input file
-t=[name]   tree file
-o=[name]   output file name (default: stdout)
-f=[number] output format
            1 = fasta
            2 = nexus
            3 = phylip (default)
            4 = msf
            5 = clustal
            6 = mega
            7 = pir
            8 = mega sequential
            9 = phylip sequential
            10 = paml
-e=[name]   error file name
-l          list the models and modifiers
-m=[name]   model name
-mf=[name]  model factories
-p          prediction
-c          codon
-a          translation
-n          nucleotide
-uselengths use branch lengths
-prunetree  prune tree to match alignment
-prunealn   prune alignment to match tree
-shortnames truncate names at first space
-quiet      no screen output
-noxpost    do not expand alignment in post
-dots       show progress while calculating
-gtr        use GTR model
-kappa=[n]  fixed kappa value
-eqfreq     use equal base frequencies
-emfreq     use empirical base frequencies
-fixedfreq  use specified base frequencies
-noadjustbl do not adjust branch lengths
-termgap    penalty for gaps at end of sequences
-nomemsave  do not save memory (default: save memory if possible)
-showtrees  write intermediate trees
-showall    write intermediate alignments
-showevery  write intermediate every n steps (default 1)
-showpost   write posterior probabilities instead of MAP
-showdiffs  write MAP alignment marking differences
-showanc    write ancestral alignments
-showtransf write codon translation alignment
-showxml    write output in BFP XML format
-showxmldna write output in BFP XML format (DNA only)
-showmafa   write output in multiple alignment format
-showfasta  write output in fasta format
-showphylip write output in phylip format
-showmsf    write output in msf format
-showclustal write output in clustal format
-showmega   write output in mega format
-showpir    write output in pir format
-showmegas  write output in mega sequential format
-showphyls  write output in phylip sequential format
-showpaml   write output in paml format
-showtreeformat write output in phylip tree format
-showtreenewick write output in newick tree format
-showtreenexus write output in nexus tree format
-showtreeapx write output in apx tree format
-showtreeall write output in all tree formats
-showtreeevery write output in all tree formats every n steps
-showtreeprune write output in prune tree format
-showtreeprunealn write output in prune tree and alignment formats
-showtreeprunealnall write output in all prune tree and alignment formats
-showtreeprunealnevery write output in all prune tree and alignment formats every n steps
-showtreeprunealnfactor=[n] write output in prune tree and alignment formats every n * factor steps
-showtreeprunealnfactorall=[n] write output in all prune tree and alignment formats every n * factor steps
-showtreeprunealnfactorevery=[n] write output in all prune tree and alignment formats every n * factor steps
-showtreeprunealnfactorevery=[n] write output in all prune tree and alignment formats every n * factor steps
-showtreeprunealnfactorevery=[n] write output in all prune tree and alignment formats every n * factor steps
```

PRS_m

Gene.prank supports compatibility with v.131.1 or earlier(version v.170) arguments. This can be a PRS (formerly the optimizing generator), command line argument or a file where type is automatically recognized (based on the extension). Command line arguments override those in the PRS file. Unknown, non-deprecated options could be wrong and result in an error or a slow/wrong execution mode.

Additional information

List of all available keywords

```
input
    -d=[name]   input file
    -t=[name]   tree file
    input_format = fasta   input format
    -f=[number] input format
                1 = fasta
                2 = nexus
                3 = phylip (default)
                4 = msf
                5 = clustal
                6 = mega
                7 = pir
                8 = mega sequential
                9 = phylip sequential
                10 = paml
    input_strict_parsing = false   input strict parsing
    -e=[name]   error file name
    -l          list the models and modifiers
    -m=[name]   model name
    -mf=[name]  model factories
    -p          prediction
    -c          codon
    -a          translation
    -n          nucleotide
    -uselengths use branch lengths
    -prunetree  prune tree to match alignment
    -prunealn   prune alignment to match tree
    -shortnames truncate names at first space
    -quiet      no screen output
    -noxpost    do not expand alignment in post
    -dots       show progress while calculating
    -gtr        use GTR model
    -kappa=[n]  fixed kappa value
    -eqfreq     use equal base frequencies
    -emfreq     use empirical base frequencies
    -fixedfreq  use specified base frequencies
    -noadjustbl do not adjust branch lengths
    -termgap    penalty for gaps at end of sequences
    -nomemsave  do not save memory (default: save memory if possible)
    -showtrees  write intermediate trees
    -showall    write intermediate alignments
    -showevery  write intermediate every n steps (default 1)
    -showpost   write posterior probabilities instead of MAP
    -showdiffs  write MAP alignment marking differences
    -showanc    write ancestral alignments
    -showtransf write codon translation alignment
    -showxml    write output in BFP XML format
    -showxmldna write output in BFP XML format (DNA only)
    -showmafa   write output in multiple alignment format
    -showfasta  write output in fasta format
    -showphylip write output in phylip format
    -showmsf    write output in msf format
    -showclustal write output in clustal format
    -showmega   write output in mega format
    -showpir    write output in pir format
    -showmegas  write output in mega sequential format
    -showphyls  write output in phylip sequential format
    -showpaml   write output in paml format
    -showtreeformat write output in phylip tree format
    -showtreenewick write output in newick tree format
    -showtreenexus write output in nexus tree format
    -showtreeapx write output in apx tree format
    -showtreeall write output in all tree formats
    -showtreeevery write output in all tree formats every n steps
    -showtreeprune write output in prune tree format
    -showtreeprunealn write output in prune tree and alignment formats
    -showtreeprunealnall write output in all prune tree and alignment formats
    -showtreeprunealnevery write output in all prune tree and alignment formats every n steps
    -showtreeprunealnfactor=[n] write output in prune tree and alignment formats every n * factor steps
    -showtreeprunealnfactorall=[n] write output in all prune tree and alignment formats every n * factor steps
    -showtreeprunealnfactorevery
```

scribjet

Model editing with Scyllator

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Author(s)

- Author: Oldfield Richard
- Author: Oldfield Richard Anthony

Purpose

Scyllator can be used to improve a molecular replacement model using additional information hosted from an aligned source structure. It is based on an algorithm implemented in Schwarzenbacher et al. (2004).

See also

Scyllator is part of phenix ensemble have been superseded by phenix.ayuda ensemble

Conventions

The following terms are used with the special meaning:

- **target**: the structure to be edited
- **source**: the structure which is used as a template for the edit

Usage

Scyllator can be run from the PHENIX GUI and the command line, the only difference being the way commands are taken from the user.

Scyllator requires two sets of inputs, which are specified above as part of the main window (the frequently used options) or through a series of dialog boxes (under **Settings Set**):

- Main (main window)
- Alignment (alignment)
- Preprocessing
- Protein chains
- Nucleic acids
- Non-macromolecular
- Sequence similarity
- Pruning

Inputs can be specified in the **PDB** file input box, while alignments and target sequences can be added through the Sequence alignment tabs, and the Sequence tab, respectively. Using Source sequence,

Input files

- **Structure** (mandatory): The structure to be modified. Specific parts can be selected using PDB atom selection syntax, and the output will be combined with the unselected parts of the structure, preserving ordering to instructions given for the appropriate chain type. Accepted formats: PDB, Reciprocal solutions, .pdb, .ent
- **Source structure** (optional): Structure from which the sequence and alignment information for the target structure is derived. This is automatically extracted with the molecular replacement output, but can be specified if the source structure is different from the one used in molecular replacement. Specific parts can be selected using atom selection syntax, aligned sections, aligned sequences, Multiple aligned files can be specified, and will be combined with the main alignment. Accepted formats: PDB, Reciprocal solutions, .pdb, .ent
- Alignments in **Target** ordering, but they can be in any order. Accepted formats: Multiple alignment files, Reciprocal solutions, .aln, .msf, .fasta, .seq, .pir, .ali, .txt, .log, .out, .stdout, .stderr, .pir, .ali, .fasta, .seq, .msf, .aln, .txt, .log, .out, .stdout, .stderr
- Target sequence: Sequence to be added to the structure, accepted formats: Sequence files, .seq, .fasta, .txt, .log, .out, .stdout, .stderr
- Source sequence: Sequence from which the target sequence is derived, accepted formats: Sequence files, .seq, .fasta, .txt, .log, .out, .stdout, .stderr

Output files

By default, mode, the main processed structure is saved. The file name is generated using the following convention: run_dir_pdb_chain.pdb, where run is your defined parameter (separately from the output root), run is a number, dir is the directory, pdb is the pdb code, and chain is the chain. Other output files are generated, and are described in the relevant sections below. Output files are:

Outline of the procedure

Scyllator operates on a single chain, which can be independently configured. There are listed in order of importance for a successful alignment and with the corresponding defaults, see the Additional information section.

Preprocessing

- source=<chain> selects a subset of the input PDB file, using CMM atom atom selection syntax. Default: all. Source structure is used to provide the sequence and alignment information, and is also used to provide the ref. Atoms. Default: source=chain A
- ref=<chain> selects the reference chain. Default: ref=chain A

In addition, chains with the wrong element, and solvent atoms will be separated from protein chains if they are not separated by the source.

Protein chains

Detection

Protein chains have a model chain that are unlikely to improve signal in molecular replacement. This information is calculated from the alignment.

There are multiple algorithms available:

- conservation: Identifies the alignment position in the target (model chain) is aligned with a gap. For this algorithm, the alignment is assumed to be a multiple alignment.
- sequence_identity: Identifies the alignment position in the target (model chain) is aligned to a lower identity sequence. All sequences in a multiple alignment contribute to the score. Details of the sequence similarity calculation are given in the sequence similarity section below.
- conservation_and_sequence: Selects the union number of residues identified by a fractional offset as identified by conservation, and a fractional offset of the sequence identity. For example, if the offset is 0.5, the top 50% default cases are used over a much larger sequence similarity range (default 0.5).
- conservation_or_sequence: Selects the intersection number of residues identified by a fractional offset of the sequence similarity, and a fractional offset of the conservation. Default: 0.5

These algorithms can also be used together in any combination. In this case, a residue will be deleted if assigned to any of the selected algorithms.

Pruning

Residues which are in the minimum of a chain (taking results from deletion into account) to make it also contiguous are deleted.

- keep_only_deleted: Deleted residues (results from the algorithm) are not contiguous compared to another than a preset limit (determined by the minimum_length parameter) of the chain. Default: keep_only_deleted=false. Deleted residues are contiguous if they are separated by less than the minimum_length parameter. Default: minimum_length=5
- keep_only_deleted_ends: Deleted residues are contiguous if they are within the minimum_length parameter of the end of the chain. Default: keep_only_deleted_ends=false

These algorithms can also be used together in combination. In this case, a residue will be deleted if assigned to any of the selected algorithms.

Pruning

Residues in the remaining the best chains from the C_{α} atom up to which a residue selection in the model is calculated, and represented in the target.

- clear_model: Implements the algorithm published by Schwarzenbacher et al. (2004), who propose that the model should be cleared of residues that are not in the alignment. This is the default, and is the recommended option. Default: clear_model=true
- keep_model: Keeps the model as it is, and does not remove residues in the model. Default: keep_model=false

These algorithms can also be used together in combination. In this case, a residue will be deleted if assigned to any of the selected algorithms.

Nucleic acids

Detection

Nucleic acids have a model chain that are unlikely to improve signal in molecular replacement. This information is calculated from the alignment.

There are multiple algorithms available:

- sequence_identity: Identifies the alignment position in the target (model chain) is aligned with a gap. For this algorithm, the alignment is assumed to be a multiple alignment.
- conservation: Identifies the alignment position in the target (model chain) is aligned to a lower identity sequence. All sequences in a multiple alignment contribute to the score. Details of the sequence similarity calculation are given in the sequence similarity section below.

These algorithms can also be used together in any combination. In this case, a residue will be deleted if assigned to any of the selected algorithms.

Pruning

Nucleic acids have a model chain that are unlikely to improve signal in molecular replacement. This information is calculated from the alignment.

- keep_only_deleted: Deleted residues (results from the algorithm) are not contiguous compared to another than a preset limit (determined by the minimum_length parameter) of the chain. Default: keep_only_deleted=false. Deleted residues are contiguous if they are separated by less than the minimum_length parameter. Default: minimum_length=5
- keep_only_deleted_ends: Deleted residues are contiguous if they are within the minimum_length parameter of the end of the chain. Default: keep_only_deleted_ends=false

These algorithms can also be used together in combination. In this case the chain will be processed separately by each algorithm.

Pruning

Residues in the remaining the best chains from the C_{α} atom up to which a residue selection in the model is calculated, and represented in the target.

- clear_model: Implements the algorithm published by Schwarzenbacher et al. (2004), who propose that the model should be cleared of residues that are not in the alignment. This is the default, and is the recommended option. Default: clear_model=true
- keep_model: Keeps the model as it is, and does not remove residues in the model. Default: keep_model=false

These algorithms can also be used together in combination. In this case the chain will be processed separately by each algorithm.

Non-macromolecular chains

Non-macromolecular chains are assumed to be correct, and are retained in the output.

Sequence similarity calculation

Sequence similarity is calculated from the full alignment supplied (taking all present sequences into account). Sequence similarity is calculated for each residue in the target sequence, and is calculated from the averaged score of a window of residues centered on it. Insertion in each alignment is assigned a gap penalty of 1.0, and a gap extension penalty of 0.5. Gaps are treated as a new residue. The score for a residue is calculated from the sum of the substitution matrix score for each residue pair, divided by the number of residues in the window. The default substitution matrix is the BLOSUM62 matrix, and the default window size is 7, depending on the number of GOR residues which the previous non-GOR residue.

Sequence similarity calculation is configured individually for the steps that are using it.

Command line

```
phenix.scyllator [-h]
                 [-n NAME] [-o OUTPUT_ROOT]
                 [-s SOURCE_STRUCTURE] [-t TARGET]
                 [-a ALIGNMENT] [-r REFERENCE]
                 [-c CHAIN] [-d DIR]
                 [-v VERBOSE] [-q QUIET]
                 [-p PARAMETER_FILE]
                 [-m MODE]
                 [-f FORCE]
                 [-l LOG_FILE]
                 [-e ERROR_FILE]
                 [-x PDB_FILE_NAME]
                 [-y PDB_FILE_NAME]
                 [-z PDB_FILE_NAME]
                 [-w ALIGNMENT_FILE_NAME]
                 [-i SEQUENCE_FILE_NAME]
                 [-j SEQUENCE_FILE_NAME]
                 [-k SEQUENCE_FILE_NAME]
                 [-b DIRECTORY]
                 [-g DIRECTORY]
                 [-h DIRECTORY]
                 [-i DIRECTORY]
                 [-j DIRECTORY]
                 [-k DIRECTORY]
                 [-l DIRECTORY]
                 [-m DIRECTORY]
                 [-n DIRECTORY]
                 [-o DIRECTORY]
                 [-p DIRECTORY]
                 [-q DIRECTORY]
                 [-r DIRECTORY]
                 [-s DIRECTORY]
                 [-t DIRECTORY]
                 [-u DIRECTORY]
                 [-v DIRECTORY]
                 [-w DIRECTORY]
                 [-x DIRECTORY]
                 [-y DIRECTORY]
                 [-z DIRECTORY]
                 [-a DIRECTORY]
                 [-b DIRECTORY]
                 [-c DIRECTORY]
                 [-d DIRECTORY]
                 [-e DIRECTORY]
                 [-f DIRECTORY]
                 [-g DIRECTORY]
                 [-h DIRECTORY]
                 [-i DIRECTORY]
                 [-j DIRECTORY]
                 [-k DIRECTORY]
                 [-l DIRECTORY]
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                 [-v DIRECTORY]
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                 [-m DIRECTORY]
                 [-n DIRECTORY]
                 [-o DIRECTORY]
                 [-p DIRECTORY]
                 [-q DIRECTORY]
                 [-r DIRECTORY]
                 [-s DIRECTORY]
                 [-t DIRECTORY]
                 [-u DIRECTORY]
                 [-v DIRECTORY]
                 [-w DIRECTORY]
                 [-x DIRECTORY]
                 [-y DIRECTORY]
                 [-z DIRECTORY]
```

Command to execute:

```
phenix.scyllator [-h]
                 [-n NAME] [-o OUTPUT_ROOT]
                 [-s SOURCE_STRUCTURE] [-t TARGET]
                 [-a ALIGNMENT] [-r REFERENCE]
                 [-c CHAIN] [-d DIR]
                 [-v VERBOSE] [-q QUIET]
                 [-p PARAMETER_FILE]
                 [-m MODE]
                 [-f FORCE]
                 [-l LOG_FILE]
                 [-e ERROR_FILE]
                 [-x PDB_FILE_NAME]
                 [-y PDB_FILE_NAME]
                 [-z PDB_FILE_NAME]
                 [-w ALIGNMENT_FILE_NAME]
                 [-i SEQUENCE_FILE_NAME]
                 [-j SEQUENCE_FILE_NAME]
                 [-k SEQUENCE_FILE_NAME]
```

PHIL argument:

```
phenix.scyllator
```

Multiple values accepting to the scope of each keyword. It is possible to turn interpretation off based on keyword.

Rename

Remove residues exceeding their numbered in the target structure. It also "resorts" the structure, i.e. reorders the residues in the structure to be consecutive. Residues are renumbered, and the alignment is adjusted accordingly by present gaps (available as the alignment parameter after a successful run).

- rename: Rename, default: rename=false

Non-macromolecular chains

Non-macromolecular chains are assumed to be correct, and are retained in the output.

Sequence similarity calculation

Sequence similarity is calculated from the full alignment supplied (taking all present sequences into account). Sequence similarity is calculated for each residue in the target sequence, and is calculated from the averaged score of a window of residues centered on it. Insertion in each alignment is assigned a gap penalty of 1.0, and a gap extension penalty of 0.5. Gaps are treated as a new residue. The score for a residue is calculated from the sum of the substitution matrix score for each residue pair, divided by the number of residues in the window. The default substitution matrix is the BLOSUM62 matrix, and the default window size is 7, depending on the number of GOR residues which the previous non-GOR residue.

Sequence similarity calculation is configured individually for the steps that are using it.

Complications

Non-macromolecular and nucleic problems

Processing features

- Non-macromolecular chains (Non-standard chain) in conversion (nucleic) cannot be similarity aligned to the alignment, and should be discarded from the alignment.
- Non-standard chains (Non-standard chain) in conversion (nucleic) cannot be aligned and a gap being included in the model. Although this possibly indicates an error in the alignment and in alignment preparation, it is also possible that non-standard residues are present in the target. In this case, the non-standard residue is assumed to be correct, and is retained in the output.
- Non-standard chains (Non-standard chain) in conversion (nucleic) of the previous non-GOR residue (the previous non-GOR residue) will be discarded, and the residue in GOR residues (the previous non-GOR residue) will be deleted.

Error messages

- No PDB file specified there are no PDB files to process
- Source structure specified, but no source sequence specified results in an empty structure.
- Alignment in alignments have been specified, but no source sequence specified results in an empty structure.
- Source structure specified, but no source sequence specified results in an empty structure.
- Source structure specified, but no source sequence specified results in an empty structure.
- Source structure specified, but no source sequence specified results in an empty structure.
- Source structure specified, but no source sequence specified results in an empty structure.
- Source structure specified, but no source sequence specified results in an empty structure.

Warning messages

- Model and alignment length mismatch: Sometimes gap identical matching statistics and the current alignment length. This is a warning, and the alignment will be extended with gaps to match the model length. Based on the program and the order of sequences in the alignment file.
- Source structure specified, but no source sequence specified results in an empty structure: This warning is raised when sequence matching cannot be performed because the sequence length of a sequence is zero. Check the input sequence and alignment files.
- Source structure: Check and interpolate between the alignment and the chain sequence. These are sometimes gap identical matching statistics and the current alignment length. This is a warning, and the alignment will be extended with gaps to match the model length. Based on the program and the order of sequences in the alignment file.
- Source structure: Check and interpolate between the alignment and the chain sequence. These are sometimes gap identical matching statistics and the current alignment length. This is a warning, and the alignment will be extended with gaps to match the model length. Based on the program and the order of sequences in the alignment file.

References

Schwarzenbacher R(1) **The importance of alignment accuracy for molecular replacement.** J. Acta Crystallogr. D. Biol. Crystallogr. 60, 1305-10. Epub 2004 Jun 26. Schwarzenbacher, Ralph. **PMID:** 15246990

Citation

Implementation of molecular replacement models with Scyllator. R. Oldfield and R. J. Read Acta Cryst. D (2011) in preparation

Additional information

List of all available keywords

```
Macro = Root
  Root_Name = Root
  Alignment_Parameters = Alignment
    Alignment_Source_Parameters = Alignment
      Source_Alignment_Parameters = Alignment
        Source_Alignment_Parameters_Source = Alignment
        Source_Alignment_Parameters_Target = Alignment
    Alignment_Target_Parameters = Alignment
      Target_Alignment_Parameters = Alignment
      Target_Alignment_Parameters_Source = Alignment
      Target_Alignment_Parameters_Target = Alignment
  Input = Input
    Input_Structure = Input
      Input_Structure_Source = Input
      Input_Structure_Source_Source = Input
      Input_Structure_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source = Input
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      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
      Input_Structure_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source_Source = Input
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sculptor_tarn

Phenix *Python based Hierarchical Environment for Integrated Xtallography*

Model editing with Sculptor

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  - Miscellaneous options
- Output files
  - Atomic coordinate files
  - Chain matching output
- Error estimates
  - Error estimates
  - Error estimates
  -

Algorithm for text packaging

Packaging binary with

```
                                  uint64_t
                                  uint8_t
                                  uint16_t
                                  uint32_t
```

search_and_morph

Phenix *Python-based Hierarchical Environment for Integrated Xtallography*

Model searching and morphing using secondary structure matching (SSM)

Author(s)

T. Wriedt, and Joseph Tom Terwilliger

Purpose

Search and morph models in the PDB similar to a supplied model using SSM matching, superimpose the matching structures, then optionally morph them to be similar to the target model and write out the joined PDB file.

Usage

Here search_and_morph works:

Search and morph uses SSM based secondary structure matching to find structures in the PDB that are similar to a supplied model. The matching structures are then superimposed on the supplied model and optionally morphed to be similar to the supplied model. The morphing is done by moving the secondary structure elements. Where there are secondary structure elements in the supplied model and in the matching structure, these are matched and the matching structure is morphed to be similar to the supplied model. Where there are no matches, the matching structure is left unmoved.

Morphing is based on the PDB concept of homology with a 70% identity and 70% coverage as in clustalw or in the Blast and Blast2 programs. The main chain coordinates of these structures are supplied in a database as part of the PDB.

Normally the base unit of a model is a set of three pairs of secondary structure elements (they can be overlapping) and the same applied analogously to the two structures. Such a model is called a triad in the terminology of SSM.

A scanning triads yields a unique orientation of the moving model. Matching triads are grouped into sets in which the orientations are similar to one another. The PDB entries representing the largest groups are then tested for match to the target structure.

Generally if database is set to "SWISSPT", sequence neighbors of these PDB entries are identified and added to the list of matches before the SSM matching is performed.

The structures to be examined are either loaded from the Phenix database or downloaded from the PDB. They are then matched against the supplied model using SSM matching. The matching structure is then moved to the structure in the same way as in phenix.superimpose and, morph. In this procedure the best fitting secondary structure is used to define a rotation and translation. The matching structure is then changed over a typical distance of about 10 A per to the parameter distance_from_target.

Finally, optionally the moving model are trimmed to remove segments that are very different from the fixed model.

Examples

Standard run of search_and_morph:

Running search_and morph is easy. Here the command line and run look:

```
phenix.search_and_morph mol.pdb target.pdb
```

This will find structures in the PDB similar to model.pdb, superimpose them, morph them to match, and trim files for the matching regions.

Possible Problems

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
search_and_morph
  model = None                      PDB file or PHENIX SEQ: set used as command line
  target = None
    model = None                    Input PDB file to be and match
    target = None                   Input PDB file or sequence file against which to match
    trim_pdb_pdb = None             Input PDB file with trimming info (chain/resseq/ins/chain)

  output_files
    prefix = search_and_morph_prefix = None   Prefix for output filenames

  search_and_morph
    distance_from_target = 10       Distance moving atoms after superimposing
    trim = True                     Trim moving model after morphing
    matching_structure_fraction = 0.5   Fraction of matching structure (secondary structure) and
                                        matching sequence to include before morphing (0.0 to 1.0)
                                        Structures are included in descending order of the number of
                                        residues in the matching sequence or secondary structure
    minimum = 0.0001667,0.0001667,0.0   Minimum rotation and translation for the rotation to
                                        continue (default 0.0001667,0.0001667,0.0)
    number_of_cycles_to_refine = 5      Number of rigid-body refinements to search of curve.default: no 10
                                        Number of cycles to refine
                                        Number of cycles to refine
    min_match = 0.7                     Minimum fraction of matching SSM
    pdb_list_type = None                List of PDB ID or pdb ID and chain,or to include (PDB or PDB,ID
                                        or PDB,ID,chain)
    pdb_exclude_list = None             List of PDB ID or pdb ID and chain,or to exclude (PDB or PDB,ID
                                        or PDB,ID,chain)
    pdb_exclude_sequence_fraction = 0.  Include pdb PDB chains with sequence identity>=
                                        Include pdb PDB chains with sequence identity>=
                                        Include pdb PDB chains with sequence identity>=
    max_number_of_chains_to_add_from_pdb = 10   Max number of chains to add from PDB
                                        Max number of chains to add from PDB: Default is 10 for quick
                                        Max number of chains to add from PDB: Default is 10 for quick
    max_match_to_match = None           Max number of matches to match from PDB: Default is 20 for quick
                                        Max number of matches to match from PDB
    matching_sequence_cutoff = 0.5      Matching sequence cutoff: fill in deep alnum within this distance, but
                                        not beyond this distance (default 0.5)
    distance_from_sequence = 10         Distance from sequence: Include atoms within this distance, but
                                        not beyond this distance (default 10)
                                        Distance from sequence: Include atoms within this distance, but
                                        not beyond this distance (default 10)
  nproc
    nproc = 1                           Number of processors to use, if None, uses all available
    quick = False                       Run quickly
  gui
    output_dir = None                   GUI-specific parameter required for output directory
```

secondary_structure

Secondary structure restraints

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- General description
- Video Tutorial
- Graphical editor
  - Secondary structure annotations
- Stacking pairs
  - Stacking annotations
- How to obtain annotations
  - Manual input
  - Automatic annotations
- Graphical editor
- References
- List of all available keywords

General description

Secondary structure restraints are a new feature in Phenix package. These restraints is regulated by the same parameters as other restraints. Currently they are used in Phenix.refine and Phenix.real_space_refine programs. They accelerate structure reliability checks. They are expected to increase resolution.

Secondary structure restraints are stored in the model file. Phenix.pdb_interpretation is responsible for the reading and writing files. We recommend to check carefully automatic assignments of SS-elements because automatic algorithms may make wrong assignments.

Video tutorial

Secondary
Structure
Restraints
Tutorial
Phenix
Secondary structure restraints
Stacking pairs
Graphical editor
Manual input
Automatic annotations
Phenix.pdb_interpretation
Phenix.refine
Phenix.real_space_refine
Phenix.ssbond
Phenix.hydrogens
Phenix.ss_annotation
Phenix.ss_restraints
Phenix.ss_validation
Phenix.ss_manipulation
Phenix.ss_to_cif
Phenix.ss_to_pdb
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Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_pdb
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Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_cif
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_pdb
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_cif
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_pdb
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_cif
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_pdb
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_cif
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_pdb
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_cif
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_pdb
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_cif
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_pdb
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_cif
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_pdb
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_cif
Phenix.ss_to_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_ss_pdb
Phenix.ss_to_ss

secondary_structure_restraints

phenix.secondary_structure_restraints

Description

It is a tool to generate secondary structure annotation in various formats using pdb file. When HELIX/SHEET records are not available in the input file, phenix.secondary_structure_restraints can be used to generate HELIX/SHEET secondary structure. To force automatic detection of protein secondary structure elements, one needs to remove HELIX/SHEET records.

There are several methods to search protein secondary structure:

- Kabsch DSSP(KD): uses DSSP
- Ksdssp(KS): uses Kabsch-Sander DSSP binary, which gives best or similar way.
- Pyksa: pure Kabsch-Sander secondary structure implementation of Kabsch-Sander. It finds more SS elements than Kabsch-Sander DSSP, but it is not as accurate as Kabsch-Sander DSSP.
- cablam: CaBLAM uses Cα trace geometry to validate protein backbone. Since the Cα trace is more simple than full backbone, CaBLAM can be used to find secondary structure in Cα only models. CaBLAM is also faster than other methods. Secondary structure detection is based on secondary residues, another CaBLAM feature.

Output formats:

- phenix (default): PDB parameters file suitable to use with all Phenix tools except phenix.refine
- phenix.refine: PDB parameters file suitable to use with phenix.refine
- pdb: HELIX/SHEET records in PDB format
- cif: mmCIF records in mmCIF format (suitable to update a cif/mmcif file)

Command line usage examples

```
% phenix.secondary_structure_restraints model.pdb
% phenix.secondary_structure_restraints model.pdb ss_restraints.phenix_refine
% phenix.secondary_structure_restraints model.pdb ignore_annotation_in_file=True
% phenix.secondary_structure_restraints model.pdb search_method=kd_or_ksdssp model.pdb
```

GUI

Graphical user interface is currently available under phenix.refine GUI, "Refinement settings" tab, select "Use secondary structure restraints" checkbox and click "More details" button.

List of all available keywords

```
ksa_cut_points = None
filter_partners = True
output.prefix = ksdssp_cut_points_ksdssp_quiet_yes_refine_nosepar_cut
quiet = False
verbose = 0
output.suffix = None
ignore_annotation_in_file = True      ignore annotation that is present in input file
file_name
  .type = pdbstr
  .multiple = True
  .optional = True
  .help = Input PDB file or string
  .parent = "phenix.secondary_structure_restraints"
  .name = pdbstr
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .enum_parent = "phenix.secondary_structure_restraints"
  .enum_name = file_name
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = True
  .enum_optional = True
  .enum_type = pdbstr
  .enum_help = Input PDB file or string
  .enum_parent = "phenix.secondary_structure_restraints"
  .enum_name = file_name
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = True
  .enum_optional = True
  .enum_type = pdbstr
  .type = None
  .multiple = False
  .optional = True
  .help = Output file
  .parent = "phenix.secondary_structure_restraints"
  .name = output
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = None
  .multiple = False
  .optional = True
  .help = Output file
  .parent = "phenix.secondary_structure_restraints"
  .name = output_log
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = bool
  .multiple = False
  .optional = True
  .help = Search for secondary structure restraints for various ligands
  .parent = "phenix.secondary_structure_restraints"
  .name = search_for_ligands
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = int
  .multiple = False
  .optional = True
  .help = Search for secondary structure restraints for ligands longer than this value
  .parent = "phenix.secondary_structure_restraints"
  .name = search_for_ligands_min_length
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = bool
  .multiple = False
  .optional = True
  .help = Search for secondary structure restraints for ligands with more than one ring
  .parent = "phenix.secondary_structure_restraints"
  .name = search_for_ligands_with_rings
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = bool
  .multiple = False
  .optional = True
  .help = Search for secondary structure restraints for ligands with rings of size 5 or 6
  .parent = "phenix.secondary_structure_restraints"
  .name = search_for_ligands_with_5_or_6_rings
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = bool
  .multiple = False
  .optional = True
  .help = Search for secondary structure restraints for ligands with aromatic rings
  .parent = "phenix.secondary_structure_restraints"
  .name = search_for_ligands_with_aromatic_rings
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = bool
  .multiple = False
  .optional = True
  .help = Search for secondary structure restraints for ligands with bonds to rings
  .parent = "phenix.secondary_structure_restraints"
  .name = search_for_ligands_with_bonds_to_rings
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = bool
  .multiple = False
  .optional = True
  .help = Search for secondary structure restraints for ligands with rings of size 5 or 6 bonded to rings of size 5 or 6
  .parent = "phenix.secondary_structure_restraints"
  .name = search_for_ligands_with_bonds_to_5_or_6_rings
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = bool
  .multiple = False
  .optional = True
  .help = Search for secondary structure restraints for ligands with aromatic rings bonded to rings
  .parent = "phenix.secondary_structure_restraints"
  .name = search_for_ligands_with_bonds_to_aromatic_rings
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = bool
  .multiple = False
  .optional = True
  .help = Search for secondary structure restraints for ligands with bonds to rings of size 5 or 6
  .parent = "phenix.secondary_structure_restraints"
  .name = search_for_ligands_with_bonds_to_5_or_6_rings
  .expert_level = 0
  .alias = None
  .enum_value = None
  .enum_help = None
  .enum_parent = None
  .enum_name = None
  .enum_alias = None
  .enum_expert_level = None
  .enum_multiple = False
  .enum_optional = True
  .enum_type = None
  .type = bool
  .multiple = False
  .optional = True
  .help = Search for secondary structure restraints for ligands with bonds to aromatic
```

segment_and_split_map

Segmentation cryo-EM maps with segment_and_split_map

Author(s):

Ashwin Dhabaria and Jeff Hoye, Tom Goddard

Purpose:

This module segments and splits map and optionally applies symmetry with a set of two (typically cryo-EM) and combination regions of density within the asymmetric unit of the map.

Usage:

How segment_and_split_map works:

The segment_and_split_map command takes a map and optionally a region to run on segment, and split_map to split the map into separate density pieces corresponding to connected components.

The segment_and_split_map tool works best at resolutions of about 4.5 Å or better.

The segment_and_split_map command can be run from the menu or from the command line in a list and work with just the map and other options.

If one map has been averaged based on NCS symmetry and you supply a file with that NCS information (symmetry command), then the segmentation will be done separately for each copy of the asymmetric unit.

Finally, the segment_and_split_map tool will find the density in the asymmetric unit and make the small pieces into a single piece if they are within a specified distance of a larger piece.

All the maps that are written by segment_and_split_map are supersampled in each axis. This typically are all related from the original map since the step size of the maps is the grid spacing divided by 2.

Output files from segment_and_split_map:

segment_and_split_map.log (log file with output from commands 1-3)

shifted_cmap.mrc.gzip NCS expansion of map, shifted to start at (0,0,0)

shifted_pdb.pdb Input PDB file (if any), shifted to match shifted_map.cmap

free_map_no.mrc Name as shifted_map.cmap, except that unassigned regions (not the asymmetric unit of NCS) are set to zero. Useful for masking.

free_mask_no.mrc Mask showing location of NCS asymmetric unit. Supersampled on free_map_no.mrc grid and shifted to start at (0,0,0).

segment_and_split_map.info.gzip Stores the info information about the segmentation. Used in segment_and_split_map.info command to continue from the segment header.

Shifting the map to the origin

Most crystallographic maps have the origin at the corner of the index (1,1,1) grid (0,0,0), while most cryo-EM maps have the origin at the center of the grid. Chimera uses the origin of the map as the center of rotation, so it is convenient to have the origin at the center of the map. Segmentation of cryo-EM maps with Chimera is easier if the origin is at the center of the map. Segmentation of crystallographic maps with Chimera is easier if the origin is at (0,0,0). The segment_and_split_map tool shifts the origin to the center of the map if the original origin is at (0,0,0). The shifted map is written to shifted_map.cmap.gzip.

Finding the region containing the molecule

By default density greater than 0.5 times the maximum density is used as part of the entire map. This is particularly useful if the original map is very large and the molecule only takes up a small part of the map. This allows one to run the segment_and_split_map tool on the full map, and then segment the molecule without having to specify a region. The segment_and_split_map tool then shifts the origin to the center of the region and writes the shifted map to shifted_map.cmap.gzip. The shifted map can then be used for further segmentation and splitting.

Finding the NCS asymmetric unit of the map

If you provide NCS matrices describing the NCS used to average the map, then segment_and_split_map will find the asymmetric unit of the map. The NCS matrices can be provided in a file with the symmetry command. In the NCS expansion will get grouped into same copy and application is a model with the symmetry command. The segment_and_split_map tool then finds the asymmetric unit of the map and writes it to shifted_map.cmap.gzip. The shifted map can then be used for further segmentation and splitting. The segment_and_split_map tool also writes a mask showing the location of the asymmetric unit to free_mask_no.mrc. The mask is supersampled on the same grid as free_map_no.mrc and shifted to start at (0,0,0).

Special treatment of structures with very high symmetry

If your structure has high symmetry (e.g. icosahedral or dodecahedral symmetry) then the segment_and_split_map tool will run out of memory. This is due to choosing a molecular of density and identifying connected components. The segment_and_split_map tool has a special option to deal with this case. The segment_and_split_map tool then finds the asymmetric unit of the map and writes it to shifted_map.cmap.gzip. The shifted map can then be used for further segmentation and splitting. The segment_and_split_map tool also writes a mask showing the location of the asymmetric unit to free_mask_no.mrc. The mask is supersampled on the same grid as free_map_no.mrc and shifted to start at (0,0,0).

Examples

Standard run of segment_and_split_map:

segment_and_split_map.log (log file with output from commands 1-3)

segment_and_split_map.log.1 (log file with output from commands 4-6)

shifted_map.cmap.gzip (shifted map, shifted to start at (0,0,0))

free_map_no.mrc (free map, shifted to start at (0,0,0))

free_mask_no.mrc (free mask, shifted to start at (0,0,0))

segment_and_split_map.info.gzip (segmentation info, shifted to start at (0,0,0))

Possible Problems

Specific limitations and problems:

Literature

Additional information:

List of all available keywords

segment_and_split_map

segment_and_split_map [<region_spec_list>] [<split_spec_list>] [<symmetry_spec_list>] [<shift_spec_list>] [<shift_to_center_spec_list>] [<shift_to_center_of_region_spec_list>] [<shift_to_center_of_region_spec_list_2>] [<shift_to_center_of_region_spec_list_3>] [<shift_to_center_of_region_spec_list_4>] [<shift_to_center_of_region_spec_list_5>] [<shift_to_center_of_region_spec_list_6>] [<shift_to_center_of_region_spec_list_7>] [<shift_to_center_of_region_spec_list_8>] [<shift_to_center_of_region_spec_list_9>] [<shift_to_center_of_region_spec_list_10>] [<shift_to_center_of_region_spec_list_11>] [<shift_to_center_of_region_spec_list_12>] [<shift_to_center_of_region_spec_list_13>] [<shift_to_center_of_region_spec_list_14>] [<shift_to_center_of_region_spec_list_15>] [<shift_to_center_of_region_spec_list_16>] [<shift_to_center_of_region_spec_list_17>] [<shift_to_center_of_region_spec_list_18>] [<shift_to_center_of_region_spec_list_19>] [<shift_to_center_of_region_spec_list_20>] [<shift_to_center_of_region_spec_list_21>] [

```
    sqrt_w_if_gamma0bb : True      Sqrt(weight) term was part of the sum squares/cross, if Model.sqrt_w
    sqrt_w_if_y : True             Sqrt(weight) term was part of the sum squares/cross, if Model.sqrt_w
    max_gap : None                 Maximum allowed number of holes in the data, on the MCD acceptance set
    max_iter : None                Maximum allowed number of iterations
    max_per_cov_blocks : 50        Maximum number of blocks of requires to be kept in the MCD acceptance s
                                   (randomly chosen if more)
    min_cov_eff_n_times_n_features Minimum value of the best fully-eigen score to determine
    : 5                            whether enough of the support could be recovered
    min_iter : 2                   Minimum allowed number of iterations to converge
    min_obs_for_coeffs : None      Minimum number of observations per group to fit coeffs
    min_obs_per_group : 10         Minimum number of all-active obs per group to fit coeffs
    n_jobs : None                  Number of parallel jobs to run
    n_reviews_per_chapter : 50     Target number of reviews per chapter
    n_reviews_per_movie : 100      Target number of reviews per movie
    n_starts_with_removed : True   Initial starting for regularized models on removed-item-first analysis
    weight_cap_pct : 0.9           Weight on control of potential of weight on observations with extreme
                                   weights, as a percentile of the weight distribution. Weights
                                   above this percentile will be capped to this value. Set to
                                   1.0 to disable. Default: 0.99. Weights are multiplied by sqrt(
                                   weight) before the regression, so a weight of 100 corresponds
                                   to a sqrt(weight) of 10.
    weight_list : None             Weight coefficients of requires list
    weight_target : 1.0            Target sum(weight) of requires list
    max_abs_coef_scaled_cap : 10   Max coefficient on particular to requires-item from Ridge map
    n_iter : 100                   Number of iterations to run the Gibbs sampler
    initial_points_in_n_cols_mult  Initial starting point was set to numbers random when creating MCD acc
    : 10                           set. Number of times the number of
    add_weights : True             Add weights to the regression, or not. Since self
                                   .weight_power is zero, weights are
    add_weights_power : 0.5        not used. Setting weight_power to nonzero and adding requires to keep is
                                   a way to bias the model toward
    Model
    debug : False                  Verbose output
    drift_pts : None               Drift dep and half_dep and step
    drift_pts_ratio : 0.5          Drift dep ratio
    drift_pts2 : None              Force the MR updates by introducing NEW correlation with step
    reverse_time : None            Flip all interval to one
    step : 1.0                     Step size for the Gibbs sampler
    debug_level : True             Map-Bayesian debug to make sure that these changes make sense
                                   Set to 0 for no output, 1 for some output, 2 for
                                   more. The information has been changed, so is therefore not comparab
                                   le to previous runs. Set to 1 for a few lines of
                                   output, 2 for a lot of output. Default: 0.
    max_beta_abs_mult_sd : False   Control parameter for the step size to be random-clipped and only
    prior_type : 1                 Prior to apply on the step sizes
    ridge_lambda : 0.0001          Ridge lambda to add to the diagonal of the covariance of sampling coeffic
                                   ients (numerical stability, prevents
    sparse_cov_weight : None       Weight of sparsity-based penalty on cov
    sparse : 1.1                   Number of predictors to use
```

selection_editor

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

Using the Selection Editor

Contents:

- Overview
- Basic Usage
- Graphical Selection
- Known Issues

Overview

The selection editor is a uniform interface for graphically selecting groups of atoms. The editor generates the appropriate phenix.selection commands and provides a simple, standard interface that the "Find/Edit" button uses to return fields in the GUI. This interface is used to define:

- Atom groups
- Ball groups
- Rigid groups
- Nonbonded analysis options (occupancies, B-factor ranges, etc.)
- Nonbonded exclusions (specific atoms, residues, chains, etc.)

Nonbonded selections mode is the editor can be accessed in the "Found" subpanel and selected at a later time ("Load" button). It is intended for more elaborate atom selection than used from Phenix program GUI (e.g. nonbonded exclusions for specific residues, or nonbonded analysis for a specific group of atoms). Most of the time, the selection editor will be used in a more simple fashion (e.g. selecting a group of atoms for a specific purpose).

Selections are generally specified in the selection editor using the phenix.selection syntax. This syntax, intended for symbolical convenience, "fits (best) on (most) if the selections are physically sensible or if there are many selections to be specified".

The "Sequence" button opens a new window showing the sequence for the given model and any secondary structure information (helices, sheets, etc.) if it is available.

The "Model" button opens a new window for graphically selecting atoms.

It is important to note that selections can only be made for options that have been enabled in the Phenix program GUI. For example, if the "Nonbonded analysis" option is not enabled, the selection editor will not be selecting BCS groups in the selection editor. Changing options in the Phenix program GUI will dynamically update the selection editor (if it is open), but changing options in the selection editor will not update other elements. Most selections will be of greatest in the Phenix program which the selection editor is called.

Closing the selection editor will update the Phenix program GUI with the selections. This is required before running the program.

Basic Usage

The selection editor can generate two basic types of selection:

- Groups composed of the selections (e.g. helix or ligand type)

Selection
Name: Selection_1
Group: Selection_1
Selection: (chain A and resseq 1:10)
Add Selection
Delete Selection
Selections
Selection_1 (chain A and resseq 1:10)
Selection_2 (chain B and resseq 1:10)
Selection_3 (chain C and resseq 1:10)
Selection_4 (chain D and resseq 1:10)
Selection_5 (chain E and resseq 1:10)
Selection_6 (chain F and resseq 1:10)
Selection_7 (chain G and resseq 1:10)
Selection_8 (chain H and resseq 1:10)
Selection_9 (chain I and resseq 1:10)
Selection_10 (chain J and resseq 1:10)
Selection_11 (chain K and resseq 1:10)
Selection_12 (chain L and resseq 1:10)
Selection_13 (chain M and resseq 1:10)
Selection_14 (chain N and resseq 1:10)
Selection_15 (chain O and resseq 1:10)
Selection_16 (chain P and resseq 1:10)
Selection_17 (chain Q and resseq 1:10)
Selection_18 (chain R and resseq 1:10)
Selection_19 (chain S and resseq 1:10)
Selection_20 (chain T and resseq 1:10)
Selection_21 (chain U and resseq 1:10)
Selection_22 (chain V and resseq 1:10)
Selection_23 (chain W and resseq 1:10)
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Selection_751 (chain W and resseq 1:

sequence_from_map

PhageSCOPE *A Fast-Input Phenotype Management for Bacteriophage Genomics*

Guessing sequence from a map with sequence_from_map

Author(s)

- Alexandra Dima, Jaqui Tom Tarantinger

Purpose

Guessing sequence from_map will use a map to guess the sequence of a supplied segment or of segments from multiseqmap.

Usage

How sequence_from_map works:

Sequence from map searches the features in a map in the positive strand side (+strand) and in the reverse complement side (-strand) for the sequence of the segment (segment_seq).

The procedure could be summarized through:

```
Step 1: Search for the segment_seq in the +strand of the map
        If found, return the sequence
Step 2: Search for the segment_seq in the -strand of the map
        If found, return the reverse complement of the sequence
Step 3: Search for the reverse complement of the segment_seq in the +strand of the map
        If found, return the sequence
Step 4: Search for the reverse complement of the segment_seq in the -strand of the map
        If found, return the reverse complement of the sequence
Step 5: If the segment_seq is not found in any of the strands, return NA
```

Step 1 of the procedure could be summarized through:

```
Step 1.1: Search for the segment_seq in the +strand of the map
          If found, return the sequence
Step 1.2: If the segment_seq is not found, check if the segment_seq is in the +strand
          If yes, check if the segment_seq is in the +strand of the sequence
          If yes, return the sequence
          If no, check if the segment_seq is in the +strand of the reverse complement
          If yes, return the reverse complement of the sequence
          If no, return NA
```

Step 1.2 of the procedure could be summarized through:

```
Step 1.2.1: Check if the segment_seq is in the +strand of the sequence
            If yes, return the sequence
Step 1.2.2: If the segment_seq is not in the +strand of the sequence, check if the segment_seq is in the +strand of the reverse complement
            If yes, return the reverse complement of the sequence
            If no, return NA
```

Step 1.2.1 and Step 1.2.2 are similar to Step 1.1 but instead of the map, the sequence and the reverse complement of the sequence are used respectively. Step 1.2.1 and Step 1.2.2 are used because the segment_seq could be a part of the sequence and not the full sequence. Step 1.2 is used to check if the segment_seq is in the sequence or in the reverse complement of the sequence. Step 1.1 is used to check if the segment_seq is in the map. Step 1.1 is used before Step 1.2 because it is faster than Step 1.2 and if the segment_seq is found in the map, the sequence and the reverse complement of the sequence are not needed to be used.

```
If yes, check whether segments corresponding the features in the map are
        in the same order and direction as the features in the map
```

The procedure of Step 1.1 could be summarized through:

```
Step 1.1.1: Search for the first segment in the segment_seq corresponding
            to the first feature in the map
Step 1.1.2: Search for the second segment in the segment_seq corresponding
            to the second feature in the map
Step 1.1.3: Search for the third segment in the segment_seq corresponding
            to the third feature in the map
Step 1.1.4: Search for the fourth segment in the segment_seq corresponding
            to the fourth feature in the map
Step 1.1.5: Search for the fifth segment in the segment_seq corresponding
            to the fifth feature in the map
Step 1.1.6: Search for the sixth segment in the segment_seq corresponding
            to the sixth feature in the map
Step 1.1.7: Search for the seventh segment in the segment_seq corresponding
            to the seventh feature in the map
Step 1.1.8: Search for the eighth segment in the segment_seq corresponding
            to the eighth feature in the map
Step 1.1.9: Search for the ninth segment in the segment_seq corresponding
            to the ninth feature in the map
Step 1.1.10: Search for the tenth segment in the segment_seq corresponding
             to the tenth feature in the map
```

Step 1.1.1 to Step 1.1.10 are similar to Step 1.1 but instead of the map, the sequence and the reverse complement of the sequence are used respectively. Step 1.1.1 to Step 1.1.10 are used because the segment_seq could be a part of the sequence and not the full sequence. Step 1.1.1 to Step 1.1.10 are used to check if the segment_seq is in the sequence or in the reverse complement of the sequence. Step 1.1 is used to check if the segment_seq is in the map. Step 1.1 is used before Step 1.2 because it is faster than Step 1.2 and if the segment_seq is found in the map, the sequence and the reverse complement of the sequence are not needed to be used.

The 10 tests for the segment_sequence segments in Step 1.1 to Step 1.1.10 are the 10 first segments of the segment_seq. If the segment_seq is longer than 10 segments, the 10 first segments are used. If the segment_seq is shorter than 10 segments, the segments are used. The 10 segments are used because it is a good number of segments to check if the segment_seq is in the map. If the segment_seq is longer than 10 segments, the 10 first segments are used because it is a good number of segments to check if the segment_seq is in the map. If the segment_seq is shorter than 10 segments, the segments are used because it is a good number of segments to check if the segment_seq is in the map.

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Examples

Standard run of sequence_from_map:

```
sequence_from_map(segment_seq=segment_seq,
                  map=map_from_map_by_name,
                  multiseqmap=multiseqmap_from_map_by_name)
```

Re-sequencing and Gibbs in a one with run_seqin_sequence=True:

```
sequence_from_map(segment_seq=segment_seq,
                  map=map_from_map_by_name,
                  multiseqmap=multiseqmap_from_map_by_name,
                  run_seqin_sequence=TRUE)
```

Literature

- **Automated phrs-class model building and sequence assignment by template matching**, TO, Tarantinger, Alex Creighton of Jaqui Tom Tarantinger, 2022
- **Read model building of alpha fold.ipa in electron density maps**, TO, Tarantinger, Alex Creighton of Jaqui Tom Tarantinger, 2022
- **Rapid model building of large proteins in electron density maps**, TO, Tarantinger, Alex Creighton of Jaqui Tom Tarantinger, 2022
- **Automated phrs-class model building and sequence assignment by template matching**, TO, Tarantinger, Alex Creighton of Jaqui Tom Tarantinger, 2022

Additional information

List of all available keywords

DATA TYPES	
Data types	
Map	
MAP_FROM_FILE	Read map from file
MAP_TO_FILE	Write map to file
MAP_PLOT	Plot map
MAP_SUBSET	Subset map
Sequence	
SEQ_FROM_FILE	Read sequence from file
SEQ_TO_FILE	Write sequence to file
SEQ_PLOT	Plot sequence
SEQ_FROM_PDB_FILE	Read sequence from pdb file
SEQ_FROM_MAP	Read sequence from map
Multiseqmap	
MULTISEQ_FROM_FILE	Read multiseqmap from file
MULTISEQ_TO_FILE	Write multiseqmap to file
MULTISEQ_PLOT	Plot multiseqmap
MULTISEQ_SUBSET	Subset multiseqmap
MULTISEQ_FROM_MAP	Read multiseqmap from map
Segment	
SEGMENT_FROM_FILE	Read segment from file
SEGMENT_TO_FILE	Write segment to file
SEGMENT_PLOT	Plot segment
SEGMENT_SUBSET	Subset segment
SEGMENT_FROM_MAP	Read segment from map
Segment_sequence	
SEGMENT_SEQUENCE_FROM_FILE	Read segment sequence from file
SEGMENT_SEQUENCE_TO_FILE	Write segment sequence to file
SEGMENT_SEQUENCE_PLOT	Plot segment sequence
SEGMENT_SEQUENCE_SUBSET	Subset segment sequence
SEGMENT_SEQUENCE_FROM_MAP	Read segment sequence from map
Segment_sequence_segments	
SEGMENT_SEQUENCE_SEGMENTS_FROM_FILE	Read segment sequence segments from file
SEGMENT_SEQUENCE_SEGMENTS_TO_FILE	Write segment sequence segments to file
SEGMENT_SEQUENCE_SEGMENTS_PLOT	Plot segment sequence segments
SEGMENT_SEQUENCE_SEGMENTS_SUBSET	Subset segment sequence segments
SEGMENT_SEQUENCE_SEGMENTS_FROM_MAP	Read segment sequence segments from map
Structure	
STRUCTURE_FROM_FILE	Read structure from file
STRUCTURE_TO_FILE	Write structure to file
Multiseqmap_segment_sequence	
MULTISEQ_SEGMENT_SEQUENCE_FROM_FILE	Read segment sequence from multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_TO_FILE	Write segment sequence to multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_PLOT	Plot segment sequence from multiseqmap
MULTISEQ_SEGMENT_SEQUENCE_SUBSET	Subset segment sequence from multiseqmap
MULTISEQ_SEGMENT_SEQUENCE_FROM_MAP	Read segment sequence from multiseqmap
Multiseqmap_segment_sequence_segments	
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_FROM_FILE	Read segment sequence segments from multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_TO_FILE	Write segment sequence segments to multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_PLOT	Plot segment sequence segments from multiseqmap
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SUBSET	Subset segment sequence segments from multiseqmap
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MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_FROM_FILE	Read segment sequence segments segments segments segments segments segments segments segments segments segments from multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_TO_FILE	Write segment sequence segments segments segments segments segments segments segments segments segments segments to multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_PLOT	Plot segment sequence segments segments segments segments segments segments segments segments segments segments from multiseqmap
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SUBSET	Subset segment sequence segments segments segments segments segments segments segments segments segments segments from multiseqmap
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_FROM_MAP	Read segment sequence segments segments segments segments segments segments segments segments segments segments from multiseqmap
Multiseqmap_segment_sequence_segments_segments_segments_segments_segments_segments_segments_segments_segments_segments_segments	
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_FROM_FILE	Read segment sequence segments segments segments segments segments segments segments segments segments segments segments from multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_TO_FILE	Write segment sequence segments segments segments segments segments segments segments segments segments segments segments to multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_PLOT	Plot segment sequence segments segments segments segments segments segments segments segments segments segments segments from multiseqmap
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SUBSET	Subset segment sequence segments segments segments segments segments segments segments segments segments segments segments from multiseqmap
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_FROM_MAP	Read segment sequence segments segments segments segments segments segments segments segments segments segments segments from multiseqmap
Multiseqmap_segment_sequence_segments_segments_segments_segments_segments_segments_segments_segments_segments_segments_segments_segments	
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_FROM_FILE	Read segment sequence segments segments segments segments segments segments segments segments segments segments segments segments from multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_TO_FILE	Write segment sequence segments segments segments segments segments segments segments segments segments segments segments segments to multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_PLOT	Plot segment sequence segments segments segments segments segments segments segments segments segments segments segments segments from multiseqmap
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SUBSET	Subset segment sequence segments segments segments segments segments segments segments segments segments segments segments segments from multiseqmap
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_FROM_MAP	Read segment sequence segments segments segments segments segments segments segments segments segments segments segments segments from multiseqmap
Multiseqmap_segment_sequence_segments_segments_segments_segments_segments_segments_segments_segments_segments_segments_segments_segments	
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_FROM_FILE	Read segment sequence segments segments segments segments segments segments segments segments segments segments segments segments segments from multiseqmap file
MULTISEQ_SEGMENT_SEQUENCE_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_SEGMENTS_TO_FILE	Write segment sequence segments

```
max_start_points_to_keep(int) = 2
                    Maximum number of starting points for sequence to consider per DNA
                    fragment (default: 2)
max_extra_gap_penalty = 1
                    Maximum extra gap penalty to allow
max_gap_penalty = 5
                    Maximum gap penalty to allow
min_score(int) = 30
                    Minimum score for a fragment
min_pcnt_aln(int) = 0.5
                    Minimum percent of alignment
min_pcnt_ident(int) = 0.5
                    Minimum percent identity
min_pcnt_gap(int) = 0.5
                    Minimum percent of gaps
min_pcnt_positive(int) = 0.5
                    Minimum percent positives
min_gapless(int) = 20
                    Minimum length of a gapless
                    alignment to consider for sequence matching
mask_lowcomp = 0
                    Mask low complexity
                    regions (0=no, 1=yes, 2=yes and also mask in nucleotides in final word
                    extension)
recursion_depth = 500000000 (0-500000000)
                    Maximum depth of recursion in core algorithm (0 MAX or 500M plenty
                    for most sequences)
lcl_to_lcl_score_group = 0
                    Group lcl sequences in consecutive groups and calculate all pairwise
                    comparisons, defined as the number of sequences to compare
lcl_to_lcl(bool) = FALSE
                    Calculate pairwise comparisons between lcl sequences (default is
                    self-comparison)
max_hsp_per_frame = 10
                    If compiled in Debug mode this flag has no effect on output, otherwise
                    it limits the number of HSPs per query per subject per frame to this
                    value. Value zero means unlimited. Value greater or equal to 1 limits
                    the number of HSPs per query per subject per frame
gap_extend_regress(bool) = FALSE
                    Use gapped extension regression test
                    (default: FALSE)
gap_trigger = 27.0
                    Number of bits to trigger gapping
dbg_gap_drop_factor = 0.5
                    Debug gapped extension drop factor
                    (default: 0.5)
dbg_gap_trigger = 0.5
                    Debug gapped extension trigger
                    (default: 0.5)
dbg_gap_hsp_cutoff = 0.5
                    Debug gapped extension HSP cutoff
                    (default: 0.5)
dbg_gap_hsp_cutoff_percentage = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100)
dbg_gap_hsp_cutoff_percentage_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_nogap = 0.5
                    Percent relative drop to the HSP cutoff for gapless extension (0 to
                    100)
dbg_gap_hsp_cutoff_percentage_nogap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapless extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_nogap_nogap = 0.5
                    Percent relative drop to the HSP cutoff for gapless extension (0 to
                    100) without gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_nogap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) without gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap_gap = 0.5
                    Percent relative drop to the HSP cutoff for gapped extension (0 to
                    100) with gap in the alignment
dbg_gap_hsp_cutoff_percentage_gap
```

set_up_gui_tests

Setting up tests that can run automatically in the Phenix GUI

Author(s)

1. Alexander Urzhumtsev, Yuri Porozovtsev

Purpose

These tests can be used to make sure that programs in the GUI can run properly. They can also be used as an example of how to set up a test in the GUI for other programs.

Framework

The PHX_TESTS directory has a set of subdirectories (CRYSTALS, A_I that can be imported as projects into the Phenix GUI. Each of these directories plays a project role (or can be imported) with the "Run/run all" button and "Run/run history".

Updating the GUI tests

New projects can be added to the GUI. TESTS directory by creating them in the Phenix GUI or (or collection of projects) by copying the directory structure and files from existing directories. The directory structure is described below. Additionally, the GUI TESTS can be run from command line. The following sections describe how to set up the GUI tests, how to run them from command line, and how to add new projects to the GUI tests.

How to set up the tests

The tests are supplied with Phenix, but you have to install them and import them into the GUI to use them. Here is how:

Install the tests

Decide where you want to put the GUI_TESTS (in this example, ~/Downloads)

Go to the phenix_regression directory with GUI_TESTS (e.g.
~/phenix/modules/phenix_regression/gui/tests, or if $PHENIX is not defined, you will need to type in the full path:

```
cd $PHENIX/modules/phenix_regression/gui/tests
```

Type in the command line:

```
install_gui_tests ~/Downloads
```

This will install the GUI_TESTS directory with the right path names in ~/Downloads

Read the Phenix GUI. You might want to do the first two (without the rotation) of Jiskeng an icon so that the tip pops up. Then do the following:

- In the Phenix GUI: select "Import Project"
  - Navigate to ~/Downloads/GUI_TESTS/A_I and hit open/import
  - The directory A_I/CRYSTALS_B should appear and open/import also automatically

Run a test

You are now ready to run one or all the tests. To run just one test:

- In the Phenix GUI, select one of these projects (PROJECT_A) and go to Job History
- Select the job you want to run (JOB_1)
- The job will be selected and you can run it with "Run"

Run a group of tests

- In the Phenix GUI, select one of these projects (PROJECT_A) and go to Job History
  - Do "Run/run all" in order
  - Wait for the first job to finish (or look for any errors)
    - If the jobs will require editing "Edit" to go on, do edit stop and wait for your OK; if will run without editing "Edit" just go on. If one of the jobs goes in the RED, OR, OPEN project, fix it/see, just restart the job and go on.

Modifying the GUI_TESTS Jobs

Modifying the GUI_TESTS jobs is important since they are needed to test new versions in phenix. Japanese, Takeda labs, Berkeley people and the GUI TESTS jobs are the only ones that use the GUI. Jobs can be modified using the GUI or directly in the GUI_TESTS directory. The following sections describe how to do this using the GUI and directly. Modifying jobs with the command line, also covered in the following sections.

Details of modifying the GUI_TESTS Jobs by creating a new set of tests

Where you have a new installation that you would like to work, you can use the
~/Downloads/GUI_TESTS/PHX_packages.sh script in your GUI_TESTS directory. Script is a shell as it won't work on Win XP.

1. Get into your GUI_TESTS directory:

```
cd ~/Downloads/GUI_TESTS
```

2. Decide where your new installation package goes. The instructions here will put it in your ~/Downloads directory and you can copy it to your regression phenix_regression/packages directory:

```
mkdir ~/Downloads/packages
./PHX_packages.sh install_package ~/Downloads
```

or ~/Downloads/GUI_TESTS/ipp ~/PHENIX/modules/phenix_regression/packages/.

This will automatically put GUI TESTS as package in Downloads and if you copy it, the one in you regression directory. You can put your own customized package anywhere you like.

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

Showing information about a map file with show_map_info

Author(s):

Tom Terwilliger, Paul Adams, Tom Terwilliger

Purpose:

The module show_map_info writes a summary of the data in a map file (ccp4/mrc/imod).

Definitions of map specifications

A map file contains a box of data on a grid. The size of data may be the original box of data or it might be a smaller box cut out of the original box of data.

The grid of the original box of data is defined by a "unit cell" and gridding for a unit cell. The unit cell usually corresponds to the box of crystal and its gridding. The unit cell and gridding of the unit cell "The unit cell" refers to the unit cell of the original box of data.

The map that is present is represented as part or all of the unit cell grid. It starts at the grid point called the "origin" and includes a number of grid points along each axis (called "nx", "ny", and "nz"). The grid points are set up in a regular manner. The map that is present does not "wrap around" the unit cell, and grid points outside the map are undefined.

Example: a full map with a unit cell grid of (10, 10, 10) goes from (0, 0, 0) to (9, 9, 9) and has dimensions of (10, 10, 10).

Example: a partial map with a unit cell grid of (10,10,10) can be origin at (2, 3, 1) and a map grid of (4*, 5*, 6*). The map goes from (2, 3, 1) and (5, 7, 6).

Note: the map may be a small piece of the unit cell (usually they are of the same). The grid can be in the dimension among 1, 2, or 3 which is the number of grid points along that dimension.

A map file has a "map unit cell" which corresponds to the dimensions of the box of data that is present in the file. The map unit cell may be different than the unit cell of the full crystal, if it is present.

External origin (ORIGIN record in map file)

A map file can have an "external origin" defined. The external origin is an offset that is intended to be applied to the grid points to determine the location of the map. If a map has an external origin defined, show_map_info will print out the value.

Phenix does not generally support the external origin values. You can however shift a model file (PDB/mmCIF) and a map file by the same amount to put them into a common frame of reference, if desired.

```
phenix.shift_model to_origin map_file.ccp4 model_file.pdb
```

Wrapping of a map

Maps can be either "wrapping" or "not wrapping" (wrapping = TRUE). If you cut out a box from a periodic map, the map will be not wrapping.

If a map is periodic, then values are extrapolated. (i.e.,it is possible the map one defined and can be obtained simply by adding or subtracting integer multiples of the unit cell dimensions to any point in the map. If a map is not wrapping, then it is not. If it is not periodic, values outside the supplied map box are undefined.

In most Phenix utilities, it is assumed that CCP4 maps are non-periodic and X-ray crystallographic maps are periodic. Cryo-EM maps are assumed to be non-periodic. Maps are assumed to be wrapping only for wrapping maps.

When you run show_map_info it will tell you whether the map supports wrapping.

Standard run of show_map_info:

You can use show_map_info to summarize a map file like this:

```
phenix.show_map_info map_file.ccp4
```

This will print out information about the map and a particular grid point with:

```
phenix.show_map_info map_file.ccp4 grid_point=1,2,3
```

Possible Problems

Specific limitations and problems:

Literature

The MRC/CCP4/mrc/imod map file format is defined at http://ccp4.ac.uk/html/maps/index.html

Additional information

List of all available keywords

```
show_map_info
  .type = bool
  .help = Show
  map_file
    .type = path
    .help = Input CCP4/MRC/IMOD/MAP/EMDB map file
    .multiple = True
    .short_name = map
    .allow_wildcards = True
    .input_extension = "map"
    .input_type = map
    .output_extension = "map"
    .output_type = map
  grid_point
    .type = int(size=3)
    .help = Show information about a particular grid point with:
            grid_point=1,2,3 will show the data at grid point (1,2,3)
  ccp4_cell
    .type = bool
    .help = Show the cell of this grid point if yes. You can specify more
            than one
            Number of cells to find a common cell
            Specifies the minimum cell of Bravais\n\n\n
```

Phenix *Python based Hierarchical Environment for Integrated Crystallography*

Homology modelling using simple_homology_model

Contents

- Purposes
- Installation
- Usage
- Input files
- Output files
- Description
  - Chain-to-alignment-matching
  - Homology modelling setup
  - Homology modelling
- Command line
  - Chain-to-alignment-matching: -ctoa argument
  - Homology modelling: -hm argument
- Examples
  - Basic usage
  - Chain-to-alignment-matching
  - List of available keywords

Purposes

This program can be used for building a homology model for a target sequence using a template structure and an alignment.

Installation

Comes bundled with open-source Phenix, software developed in the Baker laboratory at the University of Washington, and distributed through Phenix binaries.

Usage

`simple_homology_model` is available from the command line.

Input files

- **Structure** (extensions). The template structure. Accepted formats: PDB files/gzipped extensions: `.pdb`, `.ent`.
- **Alignment** (extensions). Alignment between the target and template sequences. Accepted formats: PIR, FASTA/extensions:
  - `.ali`, `.pir`, `.alignment`.
  - `.fasta`, `.fa`, `.seq`, `.aln`, `.fasta.gz`.
  - Notes: `.ali` and `.pir` files are PIR alignments. `.fasta` and `.fa` are FASTA alignments. `.seq` and `.aln` are treated as FASTA alignments. `.fasta.gz` is a gzipped FASTA alignment. Sequences must be aligned. Gaps are allowed. Only one sequence in the alignment file must be target.

Output files

The homology model is written out as `apo.pdb` in `output.dir`.

Description

The program first attempt at creating a chain-to-alignment matching that will be used subsequently in the homology modelling. Then it performs the homology modelling using the chain-to-alignment matching. The chain-to-alignment matching can be provided by the user, or it can be created automatically by the program. In the latter case, the chain-to-alignment matching is the output of the chain-to-alignment matching step of the corresponding utility, see the manual page.

Chain-to-alignment-matching

The correct chain-to-alignment matching is performed. For more information, see the Aligner manual page.

Homology modelling setup

Before running the actual modelling, the `-nrtmpl` argument limits number of templates to both cells. Then checks the distance between single residues. If this is shorter than `-maxdist`, number of residues is between, then residues are connected. If the number of residues between single residues is more than `-maxdist`, then it is assumed to belong to other loop. After this, it includes random sequence that is not separated by long dangling end. Then it checks the number of residues in the loop. If it is shorter than `-maxloop`, then it includes the loop. Finally, it checks the ends, and depending on the `-ends` argument, it includes or not the ends. Finally, it will be checked internally, and the surviving loops will be modelled. The number of loops to be modelled can be limited with the `-nrloop` argument. See the `-hm` argument.

Homology modelling

The program uses Modeller with a minimalist loop closure algorithm (`loopmodel.loop.close`), so this does not guarantee closure of the loop. Also, the loop is loaded, flagged and set internally in order of differences (`loopmodel.loop.initialize`).

Command line

```
simple_homology_model
  -ctoa <chain_to_alignment_matching_file_name>
  -hm <homology_modelling_file_name_root_1>
  -nrtmpl <number_of_templates_1>
  -maxdist <max_dist_between_residues_1>
  -maxloop <max_loop_length_1>
  -ends <ends_1>
  -nrloop <number_of_loops_1>
  -output.dir <output_dir_1>
```

Chain-to-alignment-matching: -ctoa argument

```
$ ./mafft --help
MAFFT v7.490 (2023/Jul/28)
usage:
  mafft [options] [input]
  ...(1000lines)...
  mafft [options] [input1] [input2] [input3] [input4] [input5]
  ...(1000lines)...
  mafft [options] [input1] [input2] [input3] [input4] [input5]
  ...(1000lines)...
  mafft [options] [input1] [input2] [input3] [input4] [input5]
  ...(1000lines)...
```

PHYL arguments:

Everything on stderr is parsing with a tree(1) | a tree(1) is interpreted as a PHYL argument. This can be a PHYL Newick file (extension .nwk) or a PHYL alignment file (extension .aln). The PHYL input is automatically recognized based on the extension; directory files are expanded files are recognized automatically.

Warning and error messages

Error messages

- Illegal option: The option is not PHYL-MAFFT specified.
- Illegal arg: The argument or parameter is illegal.
- Cannot open: Cannot open the file specified.
- Fatal error: Fatal error in MAFFT-profile. Check the alignment formatting was not accepted (reason indicated in the following lines).
- Cannot fork: Cannot fork the process. Check the system resources and process.
- Cannot read: Cannot read the output of a child process. Check the system resources and process.
- Cannot write: Cannot write to a pipe. Check the system resources and process.
- Cannot locate binaries modules: The Mafft-distribution is not found.
- Cannot locate binaries modules: The Mafft-distribution is not found.
- No space: Cannot allocate memory. Check the system resources and process.
- No space: Cannot allocate memory. Although Mafft-PHYL-MAFFT-profile-multiplexing succeeds, not multiple or crashes.

Warnings

- No PHYL: No PHYL is provided. Interpreted the provided file, the first sequence from the alignment will be used as the reference.
- No PHYL: Multiple output - using only first! - Mafft-generated multiple models, and only the first one will be used.

Additional information

List of all available keywords

```
input                   :  0 or 1                   # Sequence controlling input
  inputorder            :  0 or 1                   # Write order
  original              :  0 or 1                   # Alignment file name
  inputfile             :  [str]                    # Input file name

output                  :  0 or 1                   # Sequence controlling output
  kimura                :  [int]                    # Output model file name
  ktuple                :  [int]                    # Output tree file name

  hscoreoffset          :  [int]                    # Pairwise alignment parameters
  hscoreoffset          :  [int]                    # Pairwise alignment parameters
  kimura                :  [int]                    # Pairwise alignment parameters
  ktuple                :  [int]                    # Pairwise alignment parameters
  ktuple                :  [int]                    # Pairwise alignment parameters
  ktuple
```

Phenix *Python-based Hierarchical Environment for Integrated Xtallography*

Finding NCS in chains from a PDB file with simple_nca_from_pdb

Contents

- Introduction
- Outline
  - Input parameters
  - Extracting chains from pdb file(s)
  - Selecting chains for analysis (by type, from pdb model)
  - Filtering chains
  - Chain clustering
  - Identifying NCS relationships
  - Handle frameworks and symmetry
  - Output results
  - Write out PDB representation
  - Write out NCS representation
  - Write out representation of the ensemble
  - Write out representation of the asymmetric unit (the ensemble) this situation is referenced

AutoNCS

- ainsle_no_fun_pdb: Yoni Ben-Tzion/Dr. Yuval Ben-Tzion
- Fast Alignment Search Tool/ M. Emsen Kosfeld
- Yoni Ben-Tzion/ Yoni

Purpose

- This ainsle_no_fun_pdb tool/set describes N/C in the chains in a PDB file and writes out the N/C-terminal residues to separate files, sorted, and the tooltip/set includes example files.
- Unique N/C annotations against a model

Uses for searching

How ainsle_no_fun_pdb works:

The basic steps of the ainsle_no_fun_pdb are as follows:

1. Reads input PDB files, parses ATOM and HETATM records, generates
2. Identifies end of matching segments in chains in the PDB file by sequences (per value of
3. Generates output files with the matching segments, sorted by length
4. Creates summary statistics (segments found, longest/shortest lengths, average length)
5. Supports multi-chain processing
6. Handles batches from multiple directories (recursively searches subdirectories)
7. Provides detailed logging and error handling
8. Creates organized output directory structure (preserves input directory structure)
9. Offers optional verbose mode for detailed processing information

Additional notes on how ainsle_no_fun_pdb works:

The ainsle_no_fun_pdb tool processes PDB (Protein Data Bank) files to identify and extract specific segments. The first step involves parsing the input PDB file to extract all ATOM and HETATM records, organizing them by chain identifiers and residue numbers. Next, the tool analyzes the sequence of each chain to find matching segments based on the specified criteria.

The tool supports multi-chain processing, meaning it can handle PDB files with multiple chains and process each chain independently. It maintains detailed logging throughout the process, providing information about the number of segments found, their lengths, and any errors encountered.

The output consists of PDB files containing the matching segments, sorted by length in descending order. The tool also generates summary statistics including the total number of segments found, the longest and shortest segments, and the average length. This information is crucial for quality control and analysis of the results.

Error handling is robust, with the tool gracefully handling missing files, invalid PDB formats, and other potential issues. The tool provides clear error messages and continues processing other files when encountering errors with individual files.

The tool's modular design allows for easy integration into larger bioinformatics workflows. The command-line interface supports various options for customization, including verbose mode for detailed processing information and custom output directory specification.

Performance considerations include efficient memory usage by processing one chain at a time and optimized sequence matching algorithms. The tool can handle large PDB files and multiple files in batch mode without significant performance degradation.

Quality control features include comprehensive logging, error handling, and statistical reporting. The tool provides sufficient information to verify the correctness of the extraction process and identify any potential issues with the input data.

The tool's output is designed to be compatible with downstream analysis tools, with properly formatted PDB files that can be visualized in molecular viewers or processed by other bioinformatics tools.

Examples

When running:

```
python ainsle_no_fun_pdb ainsle_no_fun_pdb.pdb
```

The following files will be produced:

- N/C-specifics written to folder ainsle_no_fun_pdb
- N/C-specifics_sorted
- N/C-specifics_sorted_by_length

Matching segments are sorted by length and written into the matching segments moved into PDB files, sorted, and placed in chain_name and residue extracted from matching segment. The ainsle tool differences in output/input:

If ainsle/no_fun/no_fun differed number of atoms the structure if one containing the ainsle chain while the other contained the no_fun chain, the ainsle chain would be:

Grouping of chains is not performed:

Alternative conformers are excluded from matching segments:

The matching is done by the residues name strings, not by the residue numbers, the atoms/numbering of residues/atoms:

The result of the first search is concatenation of N/C-terminal atoms of ainsle and no_fun N/C-atoms/segments. In the case of the ainsle chain, the N/C-terminal residues are the same as the matching segments, but for no_fun, the N/C-terminal is the matching segment and the residues extracted from the matching segment.

Other outputs

To get output in other format:

```
python ainsle_no_fun_pdb ainsle_no_fun_filetoolfile
```

Details: ainsle_no_fun_pdb analyzes the chains in these pdb and identifies any N/C-that exists. For this sample run: ainsle_no_fun_pdb ainsle_no_fun_pdb.pdb

```
Input:
  Directory: /home/ubuntu/ainsle_no_fun_pdb
  Pattern: ainsle_no_fun_pdb.pdb
  Recursive: False
  Output directory: /home/ubuntu/ainsle_no_fun_pdb/N/C-specifics
  Verbose: False
  Max workers: 4
Found 1 PDB files to process
Processing: /home/ubuntu/ainsle_no_fun_pdb/ainsle_no_fun_pdb.pdb
Parsed 1 chains from /home/ubuntu/ainsle_no_fun_pdb/ainsle_no_fun_pdb.pdb
Processing chain A (length: 1)
Processing chain B (length: 1)
Processing chain C (length: 1)
Processing chain D (length: 1)
Processing chain E (length: 1)
Processing chain F (length: 1)
Processing chain G (length: 1)
Processing chain H (length: 1)
Processing chain I (length: 1)
Processing chain J (length: 1)
Processing chain K (length: 1)
Processing chain L (length: 1)
Processing chain M (length: 1)
Processing chain N (length: 1)
Processing chain O (length: 1)
Processing chain P (length: 1)
Processing chain Q (length: 1)
Processing chain R (length: 1)
Processing chain S (length: 1)
Processing chain T (length: 1)
Processing chain U (length: 1)
Processing chain V (length: 1)
Processing chain W (length: 1)
Processing chain X (length: 1)
Processing chain Y (length: 1)
Processing chain Z (length: 1)
Processing chain 0 (length: 1)
Processing chain 1 (length: 1)
Processing chain 2 (length: 1)
Processing chain 3 (length: 1)
Processing chain 4 (length: 1)
Processing chain 5 (length: 1)
Processing chain 6 (length: 1)
Processing chain 7 (length: 1)
Processing chain 8 (length: 1)
Processing chain 9 (length: 1)
Processing chain a (length: 1)
Processing chain b (length: 1)
Processing chain c (length: 1)
Processing chain d (length: 1)
Processing chain e (length: 1)
Processing chain f (length: 1)
Processing chain g (length: 1)
Processing chain h (length: 1)
Processing chain i (length: 1)
Processing chain j (length: 1)
Processing chain k (length: 1)
Processing chain l (length: 1)
Processing chain m (length: 1)
Processing chain n (length: 1)
Processing chain o (length: 1)
Processing chain p (length: 1)
Processing chain q (length: 1)
Processing chain r (length: 1)
Processing chain s (length: 1)
Processing chain t (length: 1)
Processing chain u (length: 1)
Processing chain v (length: 1)
Processing chain w (length: 1)
Processing chain x (length: 1)
Processing chain y (length: 1)
Processing chain
```

sort_helaties

Phenix *Python-based Hierarchical Environment for Integrated Xtallography*

Sorting heteratoms

The program phenix.sort_heteratoms is a utility designed to re-order the HETATM records (heteratoms) in a PDB file according to the distance from the macromolecule. This is useful for ligand fitting, since the heteratoms in the output structure (mostly ligands) will be those that are bound molecules, presumably PDB-bound ligands. The program will also optionally remove duplicate heteratoms, which may be found in a PDB file within alternate conformations. This only is kept because it is PDB file, since the program does not deal with alternate conformations. The program will also optionally remove any heteratoms that are not bound to the macromolecule.

Note that this PDB file manipulation further modifies the contents of the model according to two rules. Historically, the program output is significantly closer to the PDB conventions than the output of phenix.refine or similar programs.

List of all available parameters

file_name = None	input file
output_file = None	
remove_duplicates = True	
keep_alternate = False	
keep_water = True	Keep water molecules (default remove since assumed when determining the bound macromolecule)
keep_hydrogens = False	Keep hydrogen atoms (default is to remove them)
distance = 10.0	
remove_bonded_non_standards = True	Remove all HETATM residues with bonds to the rest of the polymer (default keep them) Note that this may result in a large number of HETATM residues in the output file, which may be undesirable if the input file contains many ligands.
preserve_chain_id = False	Preserve the original chain identifiers (rather than assigning the default chain ID) when generating new HETATM records.
select_only = False	Only output HETATM records matching the selection criteria
sort_water_by = occupancy	Sorting of waters (by default it will sort them by the contents of the occupancy field)
set_bonded_hetatm = True	Assign CONECT records where appropriate.
ignore_selection = None	Ignore HETATM records matching this selection. Note that if both this and -s/--select are specified, the output will be those HETATM records matching the selection specified with -s/--select but not matching the selection specified with -i/--ignore.
verbose = False	
quiet = False	Suppress informational output (but still write the output file)
dry_run = False	Parse the input file and report what would be done, but do not write any output.
binary_input = False	Read input file in binary mode (for Windows compatibility)
binary_output = False	Write output file in binary mode (for Windows compatibility)
overwrite = False	Allow output file to overwrite input file
help = False	Show this help message and exit
show_defaults = False	Show all parameters and their defaults
show_hidden = False	Show hidden parameters (for developers only)
show_all = False	Show all parameters, including hidden ones
model_file_extension_list = ['.pdb', '.cif', '.mmcif', '.ent', '.pdb.gz', '.cif.gz', '.mmcif.gz', '.ent.gz']	Recognized file extensions for model files
cif_file = None	Use this as CHEMICAL DEF. CIF input to CONECT line

Phenix *Python-based Hierarchical Environment for Integrated Xtallography*

phenix.structural_domain_search

Contents

- Algorithm
- Usage
  - Important parameters
  - Output
- Command-line options
- References

Finds domains by calculating the cuts in the interaction graph, and evaluates whether the cut would correspond to a viable secondary decomposition.

Algorithm

Given a pre-calculated contact graph, and a cluster size threshold above which we consider the structure to be too large to solve a priori, we recursively enumerate minimum cuts.

The structure is divided up into chunks, and an interaction network is calculated. This is then turned into an undirected graph, with edges between chunks weighted according to the number of contacts between them. Cuts are then calculated, based on size, connectedness and contact strength, and viable domains are derived. The algorithm is described in more detail in the paper, and in the code.

Usage

The only required input to the program is a structure file (PDB/CIF), which will then be analysed. The default parameters are tuned to be reasonably fast and robust, and should work for entries in the Pdb, and also for RNA/DNA/ligand complexes.

```
phenix.structural_domain_search 1ake.pdb
```

Runtime depends on the structure size, typically 1 min for structures between 200-500 residues, and 10 min for structures up to 1000 residues.

Important parameters

- **cluster_threshold** controls how many low cuts to enumerate. Increasing this number will make the search more exhaustive, but slow down.
- **cluster_size** controls the maximum size (in terms of the requested number of cuts from found. It is probably a good idea to search for some large cuts, since the lowest cut does not always corresponds to the biologically relevant domain. For example, in a multidomain protein, the lowest cut might be between two domains, but the biologically relevant domain might be a single domain. Setting cluster_size to 0 will make the program only search cuts which are the lowest cuts in the network. Setting cluster_size to 1 will make the program search for cuts which are one cut above the lowest cuts, and so on. Setting cluster_size to 2 will make the program search for cuts which are two cuts above the lowest cuts, and so on.
- **n_cut** limits the number cuts allowed to simplify the interaction graph by pruning low connected vertices. This will make the search faster, but may miss some interesting cuts. Setting n_cut to zero turns the search more efficient, but may miss some interesting cuts. Setting n_cut to 1 is the default.
- **algorithm** the quick algorithm (default) prunes graph (single) leaves, but for more truly (especially multiple) connected components, it may miss some cuts. Setting algorithm to full will make the program try to find all cuts of a given size, but this is much slower.

Output

The program writes out the best domain decomposition for each chain, as a series of .pdb files containing the relevant domains.

Various intermediate quantities are recorded in the logfile.

References

- **Efficient Algorithms for the Problem of Enumerating Cut by Non-decreasing Weights**, L. P. Gis, R. E. Wang, and K. Ko, Algorithms **30**(8), 2007 (pdf)
- **Protein Domain Decomposition using a Graph-Theoretic approach**, Acta Cryst. D **61**(8), 1021-30, (2005)
- **An Experimental Algorithm for Finding All Minimum Cuts of Undirected Graphs Parallelizable by Karger's Method**, Wagner and A Ashburgner IEEE Transactions on Pattern Analysis and Machine Intelligence **20**, 1000-1004, (1998)
- **Protein Domain Decomposition using a graph-theoretic approach**, T. G. Ye, and R. Gabow, Bioinformatics **16**(11), 1029-38, (2000)

Command-line options

```
usage:
  phenix.find [file]
  phenix.find [file]
  [keyword=value]
  [-c "keyword"]
  [-p"phil_file"] [-v]

  [-h[keyword]]
  [-h[keyword=value]]
  [-h[keyword="value"]]
  [-h[keyword=value_1,value_2,...,value_n]]
  [-h[keyword="value_1","value_2",...,"value_n"]]
  [-h[keyword="value_1","value_2",...,"value_n"]]
  [-h[keyword="value_1","value_2",...,"value_n"
```

structure_comparison

Comparing related structures in the Phenix GUI

Author:Jeyan Mariyappa, Dorothee Liebschner, Nat Echols, Billy K. Poon, Pavel Afonine, Paul Adams

Contents

- Authors
- Introduction
- Configuration
- Handling homologous sequences
- Results
- Interacting with Coot
- Citations
- Reference

Authors

- **Programming:** Nat W. Echols, Dorothee Liebschner, Nat Echols, Billy K. Poon, Pavel Afonine, Paul Adams
- **Tutorial:** Jeyan Mariyappa

Introduction

The structure comparisons GUI is a tool for parallel validation and analysis of near-identical protein structures. Multiple structures can be compared in terms of sequence and structure. Structures can be compared in terms of degree of difference (e.g. RMSD), or in terms of similarity (e.g. number of atoms within a specified distance, sequence identity). Cryo-EM models, NMR ensembles, and alternate conformations can also be compared. The GUI allows the user to select a reference structure, and then to quickly navigate through the other structures in the list, to ensure that the reference structure is the most representative, and to identify any problems with the other structures.

The structure comparison GUI is intended for use with a set of related structures, for example a set of homologous structures, or a set of structures with a common ligand. The structures should be aligned in the same coordinate frame (Phenix Superposition). It automatically set up a new project with these data, plus "Step Output" in the main GUI window, and then launches the GUI. The GUI can also be launched from the command line using "phenix.structure_comparison" from the Phenix terminal.

Limitations

- The current phenix.wizard supported at this time. PDB/CIFF are not supported.
- Only one reference model was supported. It is planned in several ways to allow for cryo-EM and NMR ensembles.
- Only a single set of chains can be compared at a time. If you have a set of heterogeneous structures, you will need to run the comparison GUI multiple times.
- Ligands are not yet supported. Future versions will include ligand RMSD and ligand-specific comparison and will allow a reference ligand to be selected. Ligand RMSD is not yet implemented in the current version.
- Nucleic acids are not yet supported.

Video Tutorial

The tutorial video is available on the Phenix Youtube channel and covers the following topics:

- Basic overview
- Setting up the structure comparison
- Advantage of Structure Comparison vs using the PDA tutorial data

Configuration and required inputs

Multiple structures can be compared, and multiple reference structures are needed. A separate file containing a single reference structure can also be used to define the reference for comparison. It is recommended to use phenix.superpose_pdbs to align the structures before comparing them, and to use the output files from phenix.superpose_pdbs as input for the comparison. The files generated by phenix.superpose_pdbs are also suitable for this tool. Each chain in the reference structure should be present in the other structures, and should have the same chain ID. Cases of the opposite scenario, where the set contain extra, are fine (extra chains will be ignored).

Phenix - Structure comparison
Structure comparison
Reference structure
Reference chain
Reference residue
Reference atom
Reference model
Reference ligand
Reference ligand chain
Reference ligand residue
Reference ligand atom
Reference ligand model
Reference ligand alternate
Reference ligand altloc
Reference ligand occupancy
Reference ligand b-factor
Reference ligand element
Reference ligand charge
Reference ligand symbol
Reference ligand name
Reference ligand type
Reference ligand id
Reference ligand chain id
Reference ligand residue id
Reference ligand atom id
Reference ligand model id
Reference ligand alternate id
Reference ligand altloc id
Reference ligand occupancy id
Reference ligand b-factor id
Reference ligand element id
Reference ligand charge id
Reference ligand symbol id
Reference ligand name id
Reference ligand type id
Reference ligand id id
Reference ligand chain id id
Reference ligand residue id id
Reference ligand atom id id
Reference ligand model id id
Reference ligand alternate id id
Reference ligand altloc id id
Reference ligand occupancy id id
Reference ligand b-factor id id
Reference ligand element id id
Reference ligand charge id id
Reference ligand symbol id id
Reference ligand name id id
Reference ligand type id id
Reference ligand id id id
Reference ligand chain id id id
Reference ligand residue id id id
Reference ligand atom id id id
Reference ligand model id id id
Reference ligand alternate id id id
Reference ligand altloc id id id
Reference ligand occupancy id id id
Reference ligand b-factor id id id
Reference ligand element id id id
Reference ligand charge id id id
Reference ligand symbol id id id
Reference ligand name id id id
Reference ligand type id id id
Reference ligand id id id id
Reference ligand chain id id id id
Reference ligand residue id id id id
Reference ligand atom id id id id
Reference ligand model id id id id
Reference ligand alternate id id id id
Reference ligand altloc id id id id
Reference ligand occupancy id id id id
Reference ligand b-factor id id id id
Reference ligand element id id id id
Reference ligand charge id id id id
Reference ligand symbol id id id id
Reference ligand name id id id id
Reference ligand type id id id id
Reference ligand id id id id id
Reference ligand chain id id id id id
Reference ligand residue id id id id id
Reference ligand atom id id id id id
Reference ligand model id id id id id
Reference ligand alternate id id id id id
Reference ligand altloc id id id id id
Reference ligand occupancy id id id id id
Reference ligand b-factor id id id id id
Reference ligand element id id id id id
Reference ligand charge id id id id id
Reference ligand symbol id id id id id
Reference ligand name id id id id id
Reference ligand type id id id id id
Reference ligand id id id id id id
Reference ligand chain id id id id id id
Reference ligand residue id id id id id id
Reference ligand atom id id id id id id
Reference ligand model id id id id id id
Reference ligand alternate id id id id id id
Reference ligand altloc id id id id id id
Reference ligand occupancy id id id id id id
Reference ligand b-factor id id id id id id
Reference ligand element id id id id id id
Reference ligand charge id id id id id id
Reference ligand symbol id id id id id id
Reference ligand name id id id id id id
Reference ligand type id id id id id id
Reference ligand id id id id id id id
Reference ligand chain id id id id id id id
Reference ligand residue id id id id id id id
Reference ligand atom id id id id id id id
Reference ligand model id id id id id id id
Reference ligand alternate id id id id id id id
Reference ligand altloc id id id id id id id
Reference ligand occupancy id id id id id id id
Reference ligand b-factor id id id id id id id
Reference ligand element id id id id id id id
Reference ligand charge id id id id id id id
Reference ligand symbol id id id id id id id
Reference ligand name id id id id id id id
Reference ligand type id id id id id id id
Reference ligand id id id id id id id id
Reference ligand chain id id id id id id id id
Reference ligand residue id id id id id id id id
Reference ligand atom id id id id id id id id
Reference ligand model id id id id id id id id
Reference ligand alternate id id id id id id id id
Reference ligand altloc id id id id id id id id
Reference ligand occupancy id id id id id id id id
Reference ligand b-factor id id id id id id id id
Reference ligand element id id id id id id id id
Reference ligand charge id id id id id id id id
Reference ligand symbol id id id id id id id id
Reference ligand name id id id id id id id id
Reference ligand type id id id id id id id id
Reference ligand id id id id id id id id id
Reference ligand chain id id id id id id id id id
Reference ligand residue id id id id id id id id id
Reference ligand atom id id id id id id id id id
Reference ligand model id id id id id id id id id
Reference ligand alternate id id id id id id id id id
Reference ligand altloc id id id id id id id id id
Reference ligand occupancy id id id id id id id id id
Reference ligand b-factor id id id id id id id id id
Reference ligand element id id id id id id id id id
Reference ligand charge id id id id id id id id id
Reference ligand symbol id id id id id id id id id
Reference ligand name id id id id id id id id id
Reference ligand type id id id id id id id id id
Reference ligand id id id id id id id id id id
Reference ligand chain id id id id id id id id id id
Reference ligand residue id id id id id id id id id id
Reference ligand atom id id id id id id id id id id
Reference ligand model id id id id id id id id id id
Reference ligand alternate id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id
Reference ligand b-factor id id id id id id id id id id
Reference ligand element id id id id id id id id id id
Reference ligand charge id id id id id id id id id id
Reference ligand symbol id id id id id id id id id id
Reference ligand name id id id id id id id id id id
Reference ligand type id id id id id id id id id id
Reference ligand id id id id id id id id id id id
Reference ligand chain id id id id id id id id id id id
Reference ligand residue id id id id id id id id id id id
Reference ligand atom id id id id id id id id id id id
Reference ligand model id id id id id id id id id id id
Reference ligand alternate id id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id id
Reference ligand b-factor id id id id id id id id id id id
Reference ligand element id id id id id id id id id id id
Reference ligand charge id id id id id id id id id id id
Reference ligand symbol id id id id id id id id id id id
Reference ligand name id id id id id id id id id id id
Reference ligand type id id id id id id id id id id id
Reference ligand id id id id id id id id id id id id
Reference ligand chain id id id id id id id id id id id id
Reference ligand residue id id id id id id id id id id id id
Reference ligand atom id id id id id id id id id id id id
Reference ligand model id id id id id id id id id id id id
Reference ligand alternate id id id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id id id
Reference ligand b-factor id id id id id id id id id id id id
Reference ligand element id id id id id id id id id id id id
Reference ligand charge id id id id id id id id id id id id
Reference ligand symbol id id id id id id id id id id id id
Reference ligand name id id id id id id id id id id id id
Reference ligand type id id id id id id id id id id id id
Reference ligand id id id id id id id id id id id id id
Reference ligand chain id id id id id id id id id id id id id
Reference ligand residue id id id id id id id id id id id id id
Reference ligand atom id id id id id id id id id id id id id
Reference ligand model id id id id id id id id id id id id id
Reference ligand alternate id id id id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id id id id
Reference ligand b-factor id id id id id id id id id id id id id
Reference ligand element id id id id id id id id id id id id id
Reference ligand charge id id id id id id id id id id id id id
Reference ligand symbol id id id id id id id id id id id id id
Reference ligand name id id id id id id id id id id id id id
Reference ligand type id id id id id id id id id id id id id
Reference ligand id id id id id id id id id id id id id id
Reference ligand chain id id id id id id id id id id id id id id
Reference ligand residue id id id id id id id id id id id id id id
Reference ligand atom id id id id id id id id id id id id id id
Reference ligand model id id id id id id id id id id id id id id
Reference ligand alternate id id id id id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id id id id id
Reference ligand b-factor id id id id id id id id id id id id id id
Reference ligand element id id id id id id id id id id id id id id
Reference ligand charge id id id id id id id id id id id id id id
Reference ligand symbol id id id id id id id id id id id id id id
Reference ligand name id id id id id id id id id id id id id id
Reference ligand type id id id id id id id id id id id id id id
Reference ligand id id id id id id id id id id id id id id id id
Reference ligand chain id id id id id id id id id id id id id id id id
Reference ligand residue id id id id id id id id id id id id id id id id
Reference ligand atom id id id id id id id id id id id id id id id id
Reference ligand model id id id id id id id id id id id id id id id id
Reference ligand alternate id id id id id id id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id id id id id id id
Reference ligand b-factor id id id id id id id id id id id id id id id id
Reference ligand element id id id id id id id id id id id id id id id id
Reference ligand charge id id id id id id id id id id id id id id id id
Reference ligand symbol id id id id id id id id id id id id id id id id
Reference ligand name id id id id id id id id id id id id id id id id
Reference ligand type id id id id id id id id id id id id id id id id
Reference ligand id id id id id id id id id id id id id id id id id id
Reference ligand chain id id id id id id id id id id id id id id id id id id
Reference ligand residue id id id id id id id id id id id id id id id id id id
Reference ligand atom id id id id id id id id id id id id id id id id id id
Reference ligand model id id id id id id id id id id id id id id id id id id
Reference ligand alternate id id id id id id id id id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id id id id id id id id id
Reference ligand b-factor id id id id id id id id id id id id id id id id id id
Reference ligand element id id id id id id id id id id id id id id id id id id
Reference ligand charge id id id id id id id id id id id id id id id id id id
Reference ligand symbol id id id id id id id id id id id id id id id id id id
Reference ligand name id id id id id id id id id id id id id id id id id id
Reference ligand type id id id id id id id id id id id id id id id id id id
Reference ligand id id id id id id id id id id id id id id id id id id id id
Reference ligand chain id id id id id id id id id id id id id id id id id id id id
Reference ligand residue id id id id id id id id id id id id id id id id id id id id
Reference ligand atom id id id id id id id id id id id id id id id id id id id id
Reference ligand model id id id id id id id id id id id id id id id id id id id id
Reference ligand alternate id id id id id id id id id id id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id id id id id id id id id id id
Reference ligand b-factor id id id id id id id id id id id id id id id id id id id id
Reference ligand element id id id id id id id id id id id id id id id id id id id id
Reference ligand charge id id id id id id id id id id id id id id id id id id id id
Reference ligand symbol id id id id id id id id id id id id id id id id id id id id
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Reference ligand model id id id id id id id id id id id id id id id id id id id id id id
Reference ligand alternate id id id id id id id id id id id id id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id id id id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id id id id id id id id id id id id id
Reference ligand b-factor id id id id id id id id id id id id id id id id id id id id id id
Reference ligand element id id id id id id id id id id id id id id id id id id id id id id
Reference ligand charge id id id id id id id id id id id id id id id id id id id id id id
Reference ligand symbol id id id id id id id id id id id id id id id id id id id id id id
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Reference ligand alternate id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand b-factor id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand element id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand charge id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand symbol id id id id id id id id id id id id id id id id id id id id id id id id
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Reference ligand chain id id id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand residue id id id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand atom id id id id id id id id id id id id id id id id id id id id id id id id id id
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Reference ligand alternate id id id id id id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand altloc id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand occupancy id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id
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Reference ligand residue id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id
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Reference ligand model id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id
Reference ligand alternate id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id
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Reference ligand occupancy id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id id
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Reference ligand chain id id id id id id id id id id id id id id id id id id id

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Phenix

Python-based Hierarchical Environment for Integrated Extensions

structure_search

Overview

Structure_search is a tool to quickly identify structural and/or sequence homology of the input PDB file from the Protein Data Bank. It uses the MMTSB toolkit algorithms and is one tool in a suite of tools that can be accessed through the MMTSB Perl scripts. Structure_search allows a user to search for similar structures in the PDB and/or sequences in the SWISS-PROT database of these homologs.

Usage

- Identify and superpose homologs with of input.pdb
  - structure_search input.pdb
- Obtain list of structures of input.pdb and of hits found in structure of these homologs
  - structure_search -s input.pdb -o output.pdb
- Use a local PDB mirror and obtain superposed homologs of input.pdb
  - structure_search -pdbdir /path/pdb/ -s input.pdb -o output.pdb

More information can be found in Input/Output files sections below.

Input files

required input:

- **pdb_file**: the file containing the protein model of interest
- **output_file**: the file where aligned and superposed structure and sequence homologs of the input file will be written

Optional input:

- **-pdb2 filename** ("1ctf.pdb") name of file of Superfit fitted in homologous PDBs, default = false
- **-pdb_dir** directory with the source files if required
- **-pdb2_dir** directory with superposed the top 10 homologs pdb2.1xxx2xxx.ent
- **-pdbdir** directory with the local PDB mirror, default = /net/cci/pdb/data/structures/all/pdb/ if LCLSF is installed
- **-dbpassword, -pdb2** ("blast") Perform only sequence search against PDB database using Phenix' ncbiblast
- **-structure, -pdb3** Perform only structure search against PDB database using the MMTSB algorithm
- **-PDB, -STRUCTURE** Set values to use local PDB mirror instead of using RCSB server. See -pdbdir and -pdb2_dir options

Output files

In addition to output.pdbpdb, these files contains results of structure_search:

- **output.pdbpdb** Superposition of the input file and its structural homologs of with PDB structure of homologs
- **output.pdb2.1xxx2xxx.ent.superposed.log** Standard RMSD output with selected pairwise alignments
- **output.pdb2.1xxx2xxx.ent.superposed.pdb** Superposition and structure-based Needleman-Wunsch alignment of the input file and its homologs
- **pdb_fasta.out** (if pdb_search=true) The containing all ligands found in all homologs from this search
- **output.superposed.PDB.fasta** Can be found in TEMPDIR, if all sequences are provided in the program input

Using Local PDB mirror

By default structure_search uses the remote RCSB mirror of PDB files SCOP server for homologsearch processes. Alternatively, structure_search can use a local mirror of structure/sequence available. PDB_PDBDIRSTRUCTure directory name defined in the running script or passed as command line options. Alternatively, users may optimize it with the command line options -PDB, -STRUCTURE, -pdbdir, -pdb2_dir, -pdb2 options.

- **-PDB, -STRUCTURE** Set values to use local PDB mirror instead of using RCSB server. See -pdbdir and -pdb2_dir options
- **-pdbdir** directory with the local PDB mirror, default = /net/cci/pdb/data/structures/all/pdb/ if LCLSF is installed, /net/ccp4data/mirrors/pdb/divided/mmCIF. The program will fail back to using RCSB server if the specified path cannot exist.

References

Li WZ, Godzik A1, Fischer D, Lu L-F, PNAS Bioinformatics, 2003, 8:807

List of all available keywords

```
structure_search
  pdb_file          = None      Input PDB file name
  -help             = None      Keyword input manual.
                                Without input keywords, this needed for a quick sequence search
  output_prefix     = "output"  Prefix of output prefix of names
  -verbose          = false     Verbose output mode
  -output_pdb       = false     Output
  -sequence_only    = false     Do a blast search against PDB database instead of doing a
                                structure search against PDB
  -structure_only   = false     Do only a Needleman-Wunsch structure search
  -pdb2             = "blast"   Perform only sequence search against PDB database using the NCBI's
                                ncbiblast
  -dir              = true      Directory input or search (-sdir, -pdbdir, or -dir)
  -pdb2_tagged      = false     Use pdb2 tagged files for multiple sequences.
  -pdb2_dir         = false     Directory where the pdb2 files are stored if they are to be downloaded
                                from the remote server
  -pdb2_get_pdb2    = false     Get BLAST PDB output alignment or structure-based alignment, but
                                not the superposition of the input PDB and its homologs
  -pdb2_pdbdbdir    = false     Use PDBDIR/pdb2.pdb2 directory for pdb2 files
  -pdb2_pdbdbdir_dir= false     Use PDBDIR/pdb2.pdb2.dir directory for pdb2 files
  -pdb2_dir_pdb     = false     Use directory pdb2.dir/pdb2.dir/pdb2.pdb2.dir/pdb2.pdb2.dir
                                for directory of pdb2.dir files to search for sequence, default is
                                pdb2.dir/pdb2.dir
  -pdb2_dir_pdb2    = false     Use directory pdb2.dir/pdb2.pdb2 to search for homologs. If
                                -pdb2_dir_pdb2 is specified, the search will be performed in the
                                directory specified by the pdb2 keyword (default=blast). For example,
                                -pdb2 pdb2 -pdb2_dir_pdb2 will search in pdb2.dir/pdb2.pdb2
  -pdb2_pdb2.dir    = false     Use pdb2.dir/pdb2.pdb2.dir/pdb2.pdb2.dir/pdb2.pdb2.dir directory
  -pdb2_dir_pdb2.dir= false     Use pdb2.dir/pdb2.pdb2.dir/pdb2.pdb2.dir/pdb2.pdb2.dir directory
  -pdb2_pdbdir      = false     Use PDBDIR/pdb2.pdb2 directory for pdb2 files
  -structure_only   = false     Do only a structure search against the PDB database using the
                                MMTSB algorithm
  -structure_pdb    = false     Use PDBDIR/pdb2.pdb2 directory for pdb2 files
  -pdb2_tagged      = false     Use pdb2 tagged files for multiple sequences.
  -pdb2_dir         = false     Directory where the pdb2 files are stored if they are to be downloaded
                                from the remote server
  -pdb2_get_pdb2    = false     Get BLAST PDB output alignment or structure-based alignment, but
                                not the superposition of the input PDB and its homologs
  -pdb2_pdbdbdir    = false     Use PDBDIR/pdb2.pdb2 directory for pdb2 files
  -pdb2_pdbdbdir_dir= false     Use PDBDIR/pdb2.pdb2.dir directory for pdb2 files
  -pdb2_dir_pdb     = false     Use directory pdb2.dir/pdb2.dir/pdb2.pdb2.dir/pdb2.pdb2.dir
                                for directory of pdb2.dir files to search for sequence, default is
                                pdb2.dir/pdb2.dir
  -pdb2_dir_pdb2    = false     Use directory pdb2.dir/pdb2.pdb2 to search for homologs. If
                                -pdb2_dir_pdb2 is specified, the search will be performed in the
                                directory specified by the pdb2 keyword (default=blast). For example,
                                -pdb2 pdb2 -pdb2_dir_pdb2 will search in pdb2.dir/pdb2.pdb2
  -pdb2_pdb2.dir    = false     Use pdb2.dir/pdb2.pdb2.dir/pdb2.pdb2.dir/pdb2.pdb2.dir directory
  -pdb2_dir_pdb2.dir= false     Use pdb2.dir/pdb2.pdb2.dir/pdb2.pdb2.dir/pdb2.pdb2.dir directory
  -pdb2_pdbdir      
```

supersyn_and_morph

Phonix — Phon-based Phonetical Phonemic to Simplified Phonetic

Model supersyntax and morphing using secondary structure matching (SSM) (deprecated, use supersyne_models)

Author(s)

- Hartmann and Joseph Von Terwellger

Purpose

Model supersyntax and morph from model. Use secondary model the missing model to be similar to the fixed model and store back to the parts that exist.

Usage

How supersyne_and_morph works:

Supersyntax and morph uses a modification of secondary structure matching (SSM) to align the two structures. Secondary structure matching works on phonic-syntactic units. The SSM matching is the same as in phonic-syntax: with shared, the SSM matching outputs of identical sequences. Unlike phonic-syntax, the SSM matching outputs of identical sequences, and also outputs of similar sequences. Similarity is determined by the distance between the two sequences. Sequences with a distance of 0 are identical, and sequences with a distance of 1 are similar. Sequences with a distance of 2 are not similar. Sequences with a distance of 3 are similar. Sequences with a distance of 4 are similar. Sequences with a distance of 5 are similar. Sequences with a distance of 6 are similar. Sequences with a distance of 7 are similar. Sequences with a distance of

Phenix *Python-based Hierarchical Environment for Integrated Crystallography*

phenix.superpose_maps

Authors

Pavel Afonine, Tom Terwilliger

Guidelines for use

Many crystallographic maps are not fundamentally two-copies-in-one-cell maps because of reference, allowing direct comparison of corresponding features in different densities. This alone is slightly misleading because the program phenix.superpose_maps does exactly that, but it does it in a way that makes it possible to do so. The reason why this is not meaningful anyway is a unique phase ambiguity arising from the same Patterson or Fourier peaks being consistent with different relative shifts between two maps. This ambiguity can be resolved by using the same phase for both maps. This is again what phenix.superpose_maps does. These are included in the PHENIX distribution as part of the "phenix" command suite.

We recommend carefully reading about the input and output files and the command line options. However, the easiest way to start using the program is to use the Graphical User Interface (GUI).

The program can be started from the Open Grid by clicking "Superpose maps" in the "Maps" category. A PDB file and two map files are required. The program will attempt to read structure factors. Map coefficients labels will be considered automatically and written to the output maps.

The program will create a new directory named "SuperposeMaps_1", where it is the 20-20 (this applies to the current directory). Inside this directory, the program will create a PDB file and two map files (the input files will be saved the only). There can be automatically loaded into Coot or PyMOL since the program is finished running.

Caveats and known limitations

1. Crystal file names are determined automatically, this will be fixed in a future version.
2. Only one chain is used in the molecular superposition at present. The program will try to guess which chain to use based on the input PDB file, but this may not be correct in some cases.
3. Because the program does not know what kind of structure (protein, DNA/RNA, small molecule, etc) is the input PDB file, the same small molecule superposition algorithm is always applied. Because of this, the program may not work well for DNA/RNA structures, and may not work well if there are more than 3 multiple sets of maps are involved.
4. The program does not attempt to make sure that all coordinates are positive (placing the origin of the unit cell at (0,0,0)). This is not a problem for most applications.
5. Maps have a unique phase, but the phase ambiguity arising from reflections in the input models, and from the resolution of the maps, is not resolved. This is a fundamental ambiguity, and it is not resolved by superposition of two maps.
6. Because maps are phased using a known set, reconstruction of the map sources is sensitive to the resolution of the input data. Superposition of two maps with different resolutions will lead to the phase shifts depending on the resolution of the map and relative to the originals. This effect is not taken into account by phenix.superpose_maps. It is best to use the same resolution for the two maps, and to use the same resolution for all of the maps.
7. Occupancies and atomic displacements are not taken into account. Maps with very different occupancies and atomic displacements will be affected by the presence of atomic density directly related to the molecule and not protein-like. Work will be a Gaussian blurred where the map has no density.

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List of all available keywords

```
output = True
  file_name = None
  log = True
  main.ncyc
    ncyc = 1 Max                    Map coefficients in MTZ format
    ncs = 1 Max                     PDB file assigned with map_1
    MtZ = Max                       Map coefficients in MTZ format
    map_1 = Max
    map_2 = Max                     Min-cutoff (0<1) for map
    map_3 = Max                     Max-cutoff (0<1) for map_1
    d_min_1 = Max                   High resolution cutoff for map_1
    d_min_2 = Max                   High resolution cutoff for map_2
  output
    output_dir = Max
    output_prefix = Max             Prefix for output
    resolution_factor = 0.25Map and special resolution factor resolution
    MtZ_format = Input input
    overwrite = True                Enabling output overwrite
    cif_file = Max                  Use file in CIFFORMAT CIF, not used on command line
  mtz
    n_processors_max = Max
  superpose_pdbs
    superpose_pdbs_flag = Max       Selection of the target chain to fit to (optional)
    selection_delta = Max           Selection of the atoms that will be fit to in selection_flag (optional)
    selection_delta_delta = Max     Selection of the atoms that will be fit to in selection_flag (optional)
    selection_delta_flag = Max      Selection of the chain that will be used to superpose (optional
                                    selection_delta_flag must be set to use this option)
    selection_delta_flag_flag = Max Selection of the chain that will be used to superpose (optional
                                    selection_delta_flag must be set to use this option) (*.cif or*.mmcif
                                    files are supported only if iotbx.cif is installed)
    fix_chain_selection_flag = Max  Fixed chain selection for superposition
    strategy = Max                  Set of strategies for superpose strategies. Default: use good for quick
                                    and good for accurate
      superpose_strategy
        use_ncs_if_available = True
        use_protein_only = True
        use_protein_chain_only = True
        remaining_atoms = rotate&shift (default)
```

superpose_models

Phenix *Python based Hierarchical Environment for Integrated Crystallography*

Model superposition with optional morphing and trimming

Author(s):

- Iversen, Andre; Oeser Carsh, Paul-Emma; Ralf W Grosse-Kunstleve, Nigel W Moriarty, Paul D Adams

Purpose

Superpose moving model on fixed model. Optionally rescale the moving model to be similar to the fixed model and trim or morph to the same that same.

Usage

Here superpose_models works:

The superpose_models tool can use either sequence based alignment with local square fitting or SSM based superposition and optional morphing.

LCQ fitting (sequence based alignment and least squares fitting)

The LCQ fitting method consists of least squares superposition of two selected parts from pdb files. If no selection is given, the whole pdb files are superposed. The selection is made by the keywords fixed_selection and moving_selection. The number of residues in fixed and moving should be different since the residue numbers are used to align the two selections. If the residue numbers are identical, the selection is made by residue name and the number of residues in the selection must be identical. The sequence alignment is then only used to find the correct order of the selected residues. The selection syntax is the same as for other phenix programs and PhenixExpert and PhenixGui are helpful in creating the selections.

SSM matching

SSM matching is secondary structure matching based similarity of secondary structure in the two models. Secondary structure elements are represented by vectors and the matching is based on the similarity of these vectors. Secondary structure elements are matched if the distance between the vectors is below a cutoff. The matching procedure is then used to find a consistent set of matches. Superposition of the two models is then done by least squares fitting of the matched secondary structure elements. The matching is very robust and fast.

A scattering cutoff(default 3.0) allows scattering of the moving model. Matching models are generated into pdb files and the best matching model is superposed. The matching models are generated in descending order of quality and each model for which the rms gives rise to a superposition that the moving model and the fixed model are within the cutoff is written to the fitted pdb superposition.

Options

- Morphing: This is the default superposition method.

  SSM matching. This is an alternative to LSQ fitting. It can be useful if your models do not have similar sequences.

  Morphing: Morphing of the superposed moving model can be accomplished by calculation of a sum weighted difference field that changes each a crystal distance of about 10 A left to the unmodified moving model. The sum weight is a Gaussian function of the distance between the moving and fixed atoms. Morphing can be carried out repeatedly by supplying a cutoff reduction in the morphing model.

  Trimming: The superposed (and optionally morphed) moving model can be trimmed to remove residues that are outside the fixed model. Trimming is carried out by the keywords trim_moving_to_fixed and trim_moving_cutoff. The trim_moving_to_fixed keyword will remove all residues in the moving model that are further than the trim_moving_cutoff distance from any atom in the fixed model. The SSM matching of secondary structure elements in the fixed model, should result in partial cut and matches and therefore incomplete secondary structure elements in the trimmed moving model. The default trim_moving_cutoff is 3.0 A.

  Rock fitting: This can be used to check superposition robustness. Random rotations and shifts of the moving model will be applied to force the target model to superpose to. You can also supply a number of rock fitting cycles using rock_fitting_cycles (default 10) and a rock_fitting_cutoff (default 0.5) to control trimming or morphing.

Examples

Standard use of superpose_models:

The superpose_models is called from the command line as:

```
phenix.superpose_models fixed_pdbfile moving_pdbfile
phenix.superpose_models fixed_pdbfile moving_pdbfile -w
```

This will superposition moving_model.pdb on fixed_model.pdb, rotate moving_model.pdb to the original orientation and write the chain and rt output, and trim moving_model.pdb to the region where they are similar and write the output to fitted_moving_model.pdb.

```
phenix.superpose_models fixed_pdbfile moving_pdbfile -w -m
```

This will find better and similar 3-mer-loop-pair and superpose moving_model.pdb on these secondary structure elements.

Possible Problems

Specific limitations and problems:

- Cryst1 records are ignored in PDB files. If cryst1 is detected, fixed and selected, moving can lead to errors if crystallographic alignment is not successful.
- Only the first model in PDB files is supported with MODEL/ENDMDL is not supported.

Literature

Additional information

List of all available keywords

```
ow_trim = None                    Ow trim or MMDB2 SEL, not used or command line
show_rms
  show_rms = None                 Calc fixed RMS rms
  fixed_selection = None          If specified, only include selected part of fixed model
  moving_selection = None         If specified, only include selected part of moving model
  moving_selection2 = None        If specified, only include selected part of moving model
  other_pdbf_to_apply = None      If specified, transform this model with the same parameters as the moving model
  write_fitted_pdb = True         Write fitted moving model to file fitted_moving_model.pdb
  only_include_first_chain = True Only use first chain in each input model
output_files
  output_prefix_suffix = Optional output prefix
  rootname_prefix = None          Prefix for all output files
  rootname_suffix = None          Suffix for all output other files
  write_log = True
  quiet = False                   Minimum text to screen(warning,error,progress if from command line)
  write_parameters_only = True    Nothing huge expected (rms). Restriction will be ignored by this flag
  overwrite = True                Rewrite or no rewrite
superpose_models
  superpose = True                Superpose moving model on fixed model
  write = True                    Write superposed moving model to file
  trim = True                     Trim moving model after morphing
  calpha_only = True              CAB models by default(include full CAB)
  ssm_matching = False            Use SSM matching
  trim_calpha_cutoff_for_ssm = 3.0 Max dist cutoff for trimming in SSM matching
  ssm_trim_cutoff = 3.0           Max value for atom filter in ssm fitting if selected
  ssm_fitting_cutoff = 3.0        Max value for fitting in ssm fitting if selected
                                  Morphing method: Morph(morph) or Morph and Rock(morph_rock) morph_method = morph
  morph_cutoff = 3.0              Max value for morphing if selected morph_method = morph
  morph_cutoff_reduction = 0.5    Cutoff reduction factor for each cycle morph_method = morph
  rock_fitting_cycles = 10        Number of rock fitting cycles if selected rock_fitting_cutoff = 0.5
  rock_fitting_cutoff = 0.5       Max value for rock fitting if selected rock_fitting_cycles = 10
  trim_moving_to_fixed = True     Include lower-quality matching(matching MMM)
  trim_moving_cutoff = 3.0        Trim by matching first if rms and sum are lower (include matching MMM)
  fix_cutoff_independent_of_rms = False
  write_model_quality = False     Write model quality to output model file(b-factor)
  write_fitted_moving_model = True Write fitted moving model to file fitted_moving_model.pdb
  write_log = True                Write log file fitted_moving_model.log
                                  Output method for output model(pdb, mmcif, mmtbf, mmtbf_gzip) output_model_format = pdb
                                  Output method for log file(stdout, log) output_log_format = log
  output_model_format = pdb       Output method for output model
  output_log_format = log         Output method for log file
  identify_superpose_profile = None Identify superpose profile(ssm_fitting_cutoff_vs_rms_cutoff)
                                  Use all parameters for superpose alignment. Defaults are good for most cases
  alignment
    alignment_method = local global
    gap_extend = 0.1
    gap_initialize = 0.9
    gap_initialize_penalty = 0.1
    local_fitting_method = least_squares
  ssm
    ssm = 1.1                     Number of alignments to use if None, uses all available
    ssm_specific_parameter = None Ssm specific parameter required for output directory
```

PHENIX *Python Hierarchical Environment for Integrated Crystallography*

Superimposing two PDB files with superpose_pdbs (deprecated, use superpose_models)

Author(s)

- Ralf Grosse-Kunstleve, Peter Zwart, Paul Adams, Nat W Grosse-Kunstleve

Purpose

superpose_pdbs is a command line tool for superimposing one PDB model on another and writing out the superimposed model.

Usage

How superpose_pdbs works:

superpose_pdbs performs a least squares superposition of two selected pairs from two pdb files. If no selections are specified, the first two chains in each file are used. The program prints out the RMS and the superposition of the number of atoms in those and once having selected different and the RMSD matrix and translation vector. The new coordinates are written to a file with the extension PDB. The default name is the name of the first input file with the extension superposed appended to the existing rotation matrix. Alternatively the output file name can be specified on the command line. Other options are available to write out the superposition matrix, to change the selections, to change the output format and to write out the rotation matrix.

Output files from superpose_pdbs

A PDB file with filled header.

Examples

Standard run of superpose_pdbs:

Running the superpose_pdbs is easy. From the command line you can type:

```
phenix.superpose_pdbs file1.pdb model.pdb
```

Alternatively you can specify the output file name:

```
phenix.superpose_pdbs file1.pdb model.pdb output.file_name=file3.pdb name="A" selection_pair="chain A pdb name 'A'"
```

Possible Problems

Specific limitations and problems:

- Different number of atoms in selection; Email and selection; missing in case when no sequence alignment
- Selection syntax: Selection syntax is the same as with multiple or sequence alignment input to that operation.
- Alternate conformers are not PDB-compliant with MODEL/ENDMDL.

Literature

Additional information

List of all available keywords

```
output.prefix = None          Prefixes of the input names to be appended
output.suffix = None          Suffixes of the input name with no ext to be appended
output.serial_number = None   Serial number to be appended to the output file
                              name. A number with leading zeros
                              will be used.
output.serial_format = phenix.pdb  Name of the pdb or cif file. Valid values: phenix.pdb|
                                   phenix.cif|phenix.mtz|phenix.hkl|phenix.fmodel|
                                   phenix.map_coeffs
                                   The name extension is required.
superpose
  superpose_method = None
    pdb_file_name_fixed = None    Name of PDB file with model to fix
    pdb_file_name_moving = None   Name of PDB file with model to be moved
    pdb_file_name_moving_out = None  Name of output PDB file to transform with the same matrix as
                                     used for superposition
  output
    file_name = None              Name of output file (default name taken from pdb_file_name_fixed
    overwrite = True              Overwrite existing files
    target_atom_format = None     Valid values: Valid values for selections. Values are PDB|I-TASS|CA and
                                  PDB|I-TASS|CA|CB|N|O|C|CG|CD|CE|CZ|CH|OH|OG|OD|OE|OZ|OG1|OG2|OD1|OD2|
                                  OE1|OE2|OH1|OH2|NE|NZ|NH1|NH2|NE1|NE2|CG1|CG2|CD1|CD2|CE1|CE2|CZ1|CZ2|
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table_one

Generating publication content with phenix.table_one

This program is experimental and still in development! Please report any problems to help@phenix-online.org

Overview

The utility table_one.cif is a tool for generating the standard tables of crystallographic statistics required for publication. It can be used with any refinement program that produces a PDB file and a reflection file in mtz or cif format. The output is written out in a form that is easy to read and processing by other programs and utilities. Only the PDB and mtz files are required, column and ref parameters can be generated for each file.

The program recognizes the output files from most common refinement programs. However, because the multiple structure block mmCIF file is the preferred format, many crystallographers do not. The document will generally reference the CCP4 implementation of the refinement program, which is usually the most common.

Configuration

Each program has a separate set for data input. The first column and data file including X-Ray Data are required. The program will attempt to find the appropriate column if the column parameter is not specified. The program will ignore any ref parameters that the user-standard logicals present in the system. Alternatively, scripts will be set up to automatically generate the ref parameters. The program will also ignore the PDB file if the pdb_in parameter is not specified. If a file is multiple CIF files or a single directory, you may specify the directory path instead of the file name.

Generate "Table 1" for journal
Input Data
Refine Output
Output Directory:
Output Prefix:
Save file name:
Save file name:
Input Data
Input Data
Input Data

trace_and_build

Phenix *Python based Hierarchical Environment for Integrated Crystallography*

Rapid model-building with trace_and_build

Author(s)

Tom Terwilliger, Tom Terwilliger

Purpose

The tutorial trace_and_build is a tool for rapid protein model building.

Usage

How trace_and_build works:

The trace_and_build tool traces the path of a polypeptide chain by starting from itself or one density, and then adding residues one at a time to the end of the chain. It then finds its positions and builds all atoms therein.

Using trace_and_build:

Normally, you will access the functionality of trace_and_build by running the Phenix map_to_model tool in the Phenix GUI. You will need to specify the map and sequence to be used for the trace, and, optionally, the seed, and, such as the unique part of a 2-fold NCS map. Your main options are the resolution, whether to fix a number of residues at the beginning of the chain, and whether to use a previously-traced model as a starting point.

Quick map file: Usually one should provide trace_and_build with a downsampled map that approximates the unique part of the map. This will speed up the calculations. The quick map file should be the same as the map file but with a smaller grid and phases that are zero, and with amplitudes scaled to match the grid of the map.

Resolution: Specify the resolution of your map (usually the resolution attained by your half-dataset Fourier shell correlation).

Sequence file: Supply a sequence file with the sequence in sequence of the molecule(s) to be built. If cross-validation is used, the sequence file should be the full sequence.

Segments to build: you can choose to build one and only one of the longest segments that trace_and_build can find, or to build all segments longer than a specified minimum length.

Seed: Specify the seed to be used for the longest segment or most thoroughly traced chain. One difference is that with seed=yes, the number of residues to be built is limited by the length of the seed and not by the length of the chain. Another difference is that with seed=yes, the residues in the seed are not allowed to be deleted, and the residues in the seed are allowed to be replaced and deletions will be made (fix_interface_deletions=true). You can set these options in the advanced menu.

Start model: You can select an input PDB model and trace_and_build will use it as a potential interpretation of the density. The input model will be used to define the starting point for the trace and to provide a set of representative atoms. The input model will take the place of the first residue, density map that is otherwise interpreted.

Procedure used by trace_and_build

The procedure used by trace_and_build has several steps:

First, density is searched, or, when a seed is supplied, searching for regular secondary structure in the map. Regular secondary structure is identified by the presence of helices and by 2nd-order secondary structure. Optionally both directions of each segment of the fixed model (or seed) are tested, and the best one is chosen.

Then, the chain is traced by adding residues one at a time to the end of the chain. The step size is 3.8 A. At each step, the density is searched along the path of a helix or strand, and the direction of the next residue is chosen to be the one that gives the most density. The residue is then built and refined, and the following step taken.

Residues are built into density one identified using the model that is supplied or found with first. Helices, strands, and loops are identified from characteristic features of high density. Starting atoms are built in one density, and the rest of the residue is built by adding atoms in the direction of the density. Side chains are built in density only if they fit into the local density.

Residues are built in sequence, and, if sequence is supplied, then positions of CB atoms are identified from the sequence and used to decide which side chain will go with the residue. The positions of CB atoms are then guessed and refined with the main chain atoms, as needed, and side chains are built for residue CB atoms and then positions in each side chain are refined with the main chain and side chain atoms in the residue.

Since it is very hard to recognize, an error in the trace can result in a wrong turn and a wrong trace and wrong residues built. To avoid this, the trace is checked for self-consistency and for consistency with the density and with those of the 10 only model with Phenix overlap. No CB positions from the fixed model are used.

Residues are built into density and refined, and then the next residue is built. The process is repeated until a maximum number of residues is built, or until a specified minimum length of chain is built, or until the end of the density is reached. Residues are built into density and refined, and then the next residue is built.

The fixed scoring model is written out so that it superimposes on the input map.

Examples

Standard run of trace_and_build:

You can use trace_and_build to build a model based on a low-CPU map:

http://phenix.lbl.gov/tutorials/trace_and_build/trace_and_build.zip

Using trace_and_build to evaluate forward and reverse versions of a model:

You can use trace_and_build to work on one or more segments, choosing both directions:

http://phenix.lbl.gov/tutorials/trace_and_build/trace_and_build_2d_segment.zip

This will trace in your fragment(s), create forward and reverse versions, score them both, and try to build the longest segment in each direction. The output will be a set of models that can be used to see which direction is better. If the sequence is known, the best direction is clearly better if one has more sites or more residues built. If one wishes to make a decision based on the density, the best direction is the one that fits the density better.

Possible Problems

Specific limitations and problems:

Literature

- **Fast processing for reconstruction of full-atom protein models from reduced representations**, T. Terwilliger, Acta Crystallogr D (2002) 58, 1465-1471.
- **Automated main-chain model building and sequence assignment by template matching**, TC. Terwilliger, Acta Crystallogr D Biol Crystallogr (2003) 59, 1771-1783.
- **Rapid model building of alpha-helices in electron density maps**, T. Terwilliger, Acta Crystallogr D Biol Crystallogr (2000) 56, 965-972.
- **Rapid model building of beta-strands in electron density maps**, TC. Terwilliger, Acta Crystallogr D Biol Crystallogr (2000) 56, 1304-1311.

Additional information

List of all available keywords

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ipw_trim_rate_rate_rate_rate_rate_rate_rate_ref = 0.0e+0
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ipw_trim_rate_rate_rate_rate_rate_rate_rate_rate_rate = 0.0e+0
ipw_trim_rate_rate_rate_rate_rate_rate_rate_rate_rate_ref = 0.0e+0
ipw_trim_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate = 0.0e+0
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ipw_trim_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_ref = 0.0e+0
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ipw_trim_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate_rate = 0.0e+0
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ipw_trim_rate
```

trim_overlapping

Phenix *Action Issue Recursive Maintenance for Integrated Bibliography*

Trimming overlapping parts of a model

Author(s)

- Tom Terwilliger

Purpose

Remove parts of a model that overlap with another model. Useful if you have a good model for part of the your structure and want to add a new model for the remainder of the structure. Also useful if you have two good fragments model for most of your structure and it provides overlapping models from another source.

How trim_overlapping works:

Calculate the distance between each atom in your model and the nearest atom in your model that have a CA or P for nucleic acid(if there is no CA or P then the nearest atom). For a cutoff distance (default is 3.0) the atoms are accepted. If the number of atoms accepted is more than a cutoff fraction (default is 0.5) then the residue is accepted. Finally any residue that is short (default 5) and isolated (default 10) is rejected. The standard segment-to-map is also applicable.

Examples

Standard run of trim_overlapping:

Trimming the overlapping parts of a model from another model:
phenix.trim_overlapping model.pdb model2.pdb output.pdb

The out.trim.log, output.pdb is water model, in_water and delta out.log_model_trimmed.pdb

Possible Problems

Specific limitations and problems:

Literature

Additional information

List of all available keywords

```
OR,AFFX,!Rev
Rev=Rev
Rev=Rev
                    Set title to PHENIX REV, not used on command line

                    Input PDB file to fix
```

```
    mask_protection = None          # If specified, only consider internal part of mask
    mask_min_area = None            # Minimum area of mask regions
    mask_to_polys_protection = None # If specified, only allow internal part of mask_to_polys
    mask_to_polys_min_area = None   # Minimum area of mask_to_polys

output_files:
    output_file_name_prefix = None  # Output files with supplied models will begin with this prefix

tile_parameters:
    tile_size = [512, 512]          # Square tiles with this dimension, in pixels
    tile_overlap_fraction_of_length = 0.1 # Minimum length of a segment after clipping (loss of shorter)
    tile_base_shift_on = None       # Shift tiles in the second or odd(1) row/column(2)

output_options:
    write_files = True              # Write output files

gpu:
    gpu_id = None                   # GPU specific parameter required for output directory
```

Analyzing unmerged data in Phenix

Introduction

Data processing software in Phenix assumes that the input data, regardless of type or format, are already both scaled and merged to yield unique reflections. The input reflections in MTZ files can be either scalar amplitudes or intensities, or complex Bijvoet-paired amplitudes or intensities. In the case of unmerged data, other programs, and sometimes will automatically merge the data internally if necessary, discarding any information about individual measurements in the process.

A note on terminology: "unmerged" in the context means that the original individual observations, rather than a single value for each unique reflection, are present in the input data file. In the context of the manual, "**This is distinct from "unmerged" data**" means the limited sense in which "unmerged" data are used in Phenix, where the data are still merged but with additional information about individual observations in Phenix data and utilities which they are not used for calculating merging statistics.

Several utilities are available in Phenix which use unmerged intensities to calculate various data quality related statistics, including the Wilson B-factor, anisotropy, intensity statistics, twinning tests, and others. Some of these are also available in the CCP4 suite, but others are unique to Phenix. Some of the statistics are also available in Phenix for data that are not unmerged, but in this case the input data are treated as if they were unique observations, and the statistics are calculated from these. Some of the statistics are also available for data in which the reflections are not unique, but in this case the statistics are calculated from the differences between the originally reported observations in the processing logfile, and the numbers reported by Phenix.

Some of the statistics are also available for data in which reflections are not unique because they are in different settings, but the accuracy of the statistics is unknown. Some of the statistics are also available for data in which the reflections are not unique because they are in different spacegroups, but in this case the statistics are calculated from the differences between the originally reported observations in the processing logfiles and the numbers reported by Phenix.

Phenix also includes a number of utilities for manipulating unmerged data, including splitting data into random or odd/even subsets, or separating out individual sets of observations for cross-validation purposes. Some of these utilities are also available in the CCP4 suite (Aimless/Pointless), but others are unique to Phenix. Phenix processing software uses these utilities and also the code for example Aimless/Pointless.

Phenix also includes a number of utilities for manipulating unmerged data, including splitting data into random or odd/even subsets, or separating out individual sets of observations for cross-validation purposes. Some of these utilities are also available in the CCP4 suite (Aimless/Pointless), but others are unique to Phenix.

```
EMPTY/Utilities/scaling/multi-xscale.sh, and so on
```

The Phenix utilities are also available in a form which can be run from command line and the data piped to specified inconsistency, but this can be very cumbersome because of a lack of the same diagnostics.

Obtaining unmerged data

For processing Phenix software accepts some processing software, these are the methods are are familiar with:

- **mtz2**: for CrystalClear directory will contain a file in Scalepack format, ending in "_unmerged.sca", which can be read by Phenix.
- **phenix.CCPtoPhenix**: will convert CCP4 unmerged data to Phenix.
- **phenix.XDSToMTZ**: will convert XDS/XSCALE output to MTZ format, with unmerged data, if any, and also XDS/XSCALE to scale data from multiple datasets, and the Phenix utilities.

Note that unmerged Scalepack format does not include the cell unit, so symmetry needs to be supplied that is consistent with the cell used in the processing software, and the Phenix utilities will assume that the cell is consistent (actually, the cell in Phenix is taken from the Scalepack file, and the cell in CrystalClear, or particular, from the MTZ file).

Xtriage and phenix.merging_statistics

phenix.merging_statistics is a simple program to calculate the standard statistics output by most data processing software, such as resolution, completeness, R-merge, R-meas, Chi-squared, R-factor, CC1/2, R-pim and so on. It can also output the data in a form which can be plotted in Phenix or other programs. It can also output the data in a form which can be read by Phenix Xtriage, which will then perform a number of additional tests on the data, including Wilson B, anisotropy, twinning, and others. Xtriage

validation

Validation tools in *Phenix*

Contents:

- Overview
- Molprobity summary
- Geometry restraints outliers
- Validation of protein geometry
- Validation of protein contacts
- All-atom contacts
- RNA validation
- Real space correlation
- POLISHER
- References
- Suggestions for improving models

Overview

The documentation covers the use of the validation software in the Phenix GUI, which is in turn an interface to the Molprobity software suite developed by the Richardson lab, and other validation tools developed in the Phenix group. Although it is possible to run validation with only a model, we recommend including experimental data, which allows more tests to be performed and more accurate results to be obtained.

The analyses performed by Phenix include:

- identification of outliers from statistical parameters (geometry, clashes, etc.)
- identification of potential errors
- identification of alternative (preferred) rotamer conformations (side chain and peptide)
- identification of alternative (preferred) Ramachandran conformations (backbone)
- suggestions for improvements (rotamer flips, etc.)
- calculation of overall quality statistics (R-factors, etc.)
- calculation of local quality statistics (real-space correlation, B-factors, RMS deviations from neighboring residues, etc.)

Most analyses performed will be included in the final output, but the Ramachandran plot and CA/P Ramachandran geometry outliers will be detected as well. Comprehensive validation of nucleic acid structures is planned for a future release.

All of our analyses depend on well-fitted and well-refined models. Unfortunately, many models in the PDB are not well-refined, and even well-refined models may have local errors that are difficult to detect. Although we do not claim to identify all such errors, we do in some cases pick up and highlight the biggest selections. If experimental data are included, Phenix will also check for errors in the model which have a high impact on the predicted phasing.

Running validation

If you are performing refinement with the Phenix GUI, the validation will be performed automatically in parallel with the refinement, and the results will be displayed in the GUI. If you are using command-line refinement, you may also find this useful. To do this, you can use a GUI for the log, and choose the option to monitor the refinement log file. Alternately, you can use a GUI for the log, but instructed the validation tools to ignore the structure. Their parameters should be selected accordingly.

After running the validation a new window will open with the results. If experimental data were included, the first tab will contain a summary of the model statistics, including R-factors, RMS deviations, and other quality measures. Additional tabs contain the Molprobity validation, which checks for atomic properties of fitted and refined models, and real-space validation.

Molprobity summary

Most of the errors detected and shown should be absolute validation criteria (mostly specific to proteins). Set the cutoffs for the Molprobity analysis to "Rigorous" with clashes being ignored is a reasonable option. Although there are no necessarily errors, they are often unnecessarily set acceptable.

Geometry restraints outliers

Phenix, the most crystallographic software, uses the Engh and Huber (1991) standard for protein, nucleic acid, and ligand geometry. Although this is a good set of ideal values, it is not necessarily the best set for a particular structure. Phenix can optionally use a set of restraints derived from the structure being refined. Deviations are used to identify potential deviations in ideal geometry, which may indicate the presence of a local error in the model. Although this is not a perfect method, it does pick up a number of errors, particularly in centers, global geometry (such as aromatic rings), and substandard (VDW) interactions. All of these are average over a large number of structures, however, which can lead to deviations in the local ideal geometry of even correct analysis (see below).

All restraint values have an associated "sigma", or the observed standard deviation from that value in very high resolution structures. This is used to weight the restraint during refinement, large deviations (greater than 3 sigma) are considered unlikely and are ignored by default in Phenix. Although this is a good method for refinement, it can be misleading when looking for potential errors in the structure. A deviation of 3 sigma is considered to be a high value, however, it is also possible for the deviation to be perfectly correct. Although this is not a perfect method, it does pick up a number of errors, these should be proven to correct, although minimal angles and sigmas.

Validation of protein geometry

The geometry of protein chains is restricted by additional empirical observations that are not part of the crystallographic target function. These include the Ramachandran plot, which describes the preferred values of the backbone torsion angles, and the Rotamer set for side chain conformations. Although these are not absolute, they are very unlikely if they are in disfavored regions. Although there are many ways to visualize these, we have chosen to use a Ramachandran plot, which is a scatter plot of the backbone torsion angles, coloring more bad outliers in a 3D histogram.

The map of the left is divided into several sections:

- The Generalized plot, with the line on the combination of Phi (X-axis) and Psi (Y-axis). This is a combination of the Ramachandran plot for all residues, the general distribution of points is taken from the Top8000 database of high resolution protein structures. The main window displays the Ramachandran plot for the selected residue, the green dot is the current position, the red dot is the previous position, and the blue dot is the next position. The Ramachandran plot for all residues is displayed in the lower window, the current residue is highlighted in red. Clicking on a point in the Ramachandran plot will select the residue closest to that point.
- Rotamer comparisons are over the Top8000 database, and an selection for angles for a backbone dependent rotamer is considered to be a rotamer outlier if it is not in the distribution of rotamers found in the Top8000 for that residue type. The distribution of the CA-CB bond conformation is also considered, if it is not in the distribution of CA-CB bond conformations for that residue type, it is considered a CB outlier. Note that Glycine has no Rotamer or outlier based on its CB conformation, and Alanine has no Rotamer or outlier based on its CB conformation.
- Cbeta deviations are based on the distance between the CB and the ideal position, if the distance is greater than 0.25 Angstroms, it is considered a CB outlier. Note that Glycine has no Cbeta deviation.
- Peptide bond planarity, omega, which is a measure of the planarity of the peptide bond, is considered unlikely if it is greater than 30 degrees from planarity, and highlighted in the Molprobity analysis. Cis-peptides are considered unlikely, and highlighted in the Molprobity analysis, cis-proline and non-cis-proline angles.

All-atom contacts

Nonbonded interactions are an important part of the model and are analyzed and highlighted. Phenix analyses all nonbonded interactions, and highlights those that are unlikely. Although there are many ways to visualize these, we have chosen to use a 3D histogram, coloring more bad outliers in a different color. Therefore, the only nonbonds are shown in the model window, and the bad nonbonds are highlighted in a different color. Although this is not a perfect method, it does pick up a number of errors, particularly those flipping based on hydrogen bonding geometry and steriles caused by many bulkier hydrogens. These include Asn, Gln, and His flips, methyl rotations, and Met, Lys, Arg, and Pro conformations, and other steric interactions.

Since hydrogens are added, phenix probes is used to analyze the atomic contacts, all atoms contact within 0.25 Angstroms of each other are considered to be in contact, and the overlap is defined as the sum of the vdw radii minus the distance (number of Angstroms). This should be as low as possible, although a value of zero is not necessarily correct, and may be a result of a steric clash between two atoms, or an interaction, or the specially neutrons scattered hydrogen atoms which make probing difficult.

Since Cbeta is able to read the concept of flips and potentially display the contacts as dots and spheres, this information will be automatically loaded into Coot when run from Phenix. Display of the dots can be toggled using the Cbeta Validation menu, and the dots can be set to be displayed in the Cbeta Validation menu. It is usually much easier to visualize the clash if the position if hydrogens are shown as well.

RNA validation

Is very short and of a rudimentary and simple stage for RNA phenix is spelled especially from the parameters in the Molprobity. Phenix is able to read the concept of flips and potentially display the contacts as dots and Coot. Overlooked Helix. Overcentered of geometry. Jerkiness of RNA structures is an ongoing project setting PDB001, currently, Coot RNA Validation menu, and the software and Molprobity suite.

Real space correlation

This is the only part of validation that depends the crystallog diffraction data. Phenix will perform local real space correlation, and B-factor analysis, and RMS deviations from neighboring residues. This is a good way to find local errors in the model. Although this is not a perfect method, it does pick up a number of errors, particularly those flipping based on hydrogen bonding geometry and steriles caused by many bulkier hydrogens. These include Asn, Gln, and His flips, methyl rotations, and Met, Lys, Arg, and Pro conformations, and other steric interactions.

Although real space CC can be a useful indicator of poorly fit regions of a molecule, it should not be interpreted as a measure of correctness. It is very easy to fit a model into density that is consistent with the data, but incorrect. A good example is a helix, which can be fitted with a wrong register and still have reasonable density and real space CC. Although this is not a perfect method, it does pick up a number of errors, particularly those flipping based on hydrogen bonding geometry and steriles caused by many bulkier hydrogens. These include Asn, Gln, and His flips, methyl rotations, and Met, Lys, Arg, and Pro conformations, and other steric interactions.

POLISHER

Phenix POLISHER (Introduced in 2009) has been added to the Phenix GUI for comparing model quality measures to the distribution of similar PDB files. Phenix POLISHER allows the user to compare the

Phenix

Python-based Hierarchical Environment for Integrated Xtallography

Cryo-EM Validation tools in Phenix

Contents

- Overview
- Model
- Model and Data FS
- Data
- References

Overview

Phenix has various tools for validating cryo-EM maps and models. They are combined into a single tool called "Validation cryo-em" which can be run from the GUI by selecting "Validation cryo-em" under "Validation" in the "Utilities" section in the "Cryo-EM" section.

Opening the program will show a window for supplying your input files and basic settings.

You will need at least a model and one map. If you provide half maps, be sure to indicate which map is the full map and which maps are the half maps. To do so, after setting the files, you can right-click on the list of a map and select "Set as half map".

Lastly, before running the program, enter the resolution of the map.

Resolution is used in all calculations and plots. Resolution is also used in the consistency of mirror setting 1 (see below). It is also used to determine the resolution of the map to be used in the transparent and solid MM-Electrostatic maps (see below).

Resolution is optional for validating the statistics, you will get a page that summarizes all the results, as well as additional pages for more detailed information about each section.

Similar to the "Comprehensive Validation (cryo-EM)" GUI, this output window can be saved in Coot and the pages with more detail information will allow you to zoom into the more problematic areas of your structure.

and zoom in on that particular stereochemical in Coot.

The results are subdivided into several categories listed below.

- **Summary**: the phenix.mtriage statistics about the images and recommends the resolution estimates
- **FSC (Half-maps)**: this shows a graph plotting the Fourier shell coefficient curve based on the two half maps, as well as the recommended resolution based on the 0.143 cutoff.
- **FSC (Model-map)**: this shows a graph plotting the Fourier shell coefficient curve based on the full map and the model, as well as the recommended resolution based on the 0.143 cutoff.

In the pages with graphs, you can save the graph and export the data used to generate the graphs into a text file.

References

Overview of the analysis and validation of cryo-EM maps and atomic models. P.V. Adams, D.A. Keedy, L.N. Kinch, J.M. Kriegler, M.L. Mayes, A.S. Sobolev, T.C. Terwilliger, T.O. Yeates, and W.A. Hendrickson. [link](https://doi.org/10.1107/S2059798321009475)

Multivalent, more and better reference data for improved all-atom structure validation. T.C. Terwilliger, P.V. Adams, R.O. Moriarty, M.L. Williams, R.M. Jakobi, R.M. Dyer, J.S. Lewis, D.A. Keedy, L.N. Kinch, J.M. Kriegler, M.L. Mayes, T.O. Yeates, W.A. Hendrickson, and D.L. Willis. P. Rosenzweig, Protein Science 30, 207-221 (2021). [Protein Science 30, 207-221 (2021)](https://doi.org/10.1002/pro.3987)

Model

This page contains the model-related metrics with additional pages for each major metric.

Generally, clicking on a row of a table or clicking a point in the graph

will zoom in on that particular stereochemical in Coot.

The model statistics are:

- **Clashes**: the number of the structure where atoms may be too close to each other. In Coot, this is shown as red dots.
- **Rotamers**: the number of side chains in unusual rotamers, which looks at several measures based on the side chain shape.
- **Ramachandran**: the number of the C alpha angles.
- **Cbs Deviation**: the deviations are generated from CB deviations (the 0.02Å of other measures), which looks at the deviation of the CB atom from the ideal position based on the other atoms in the residue.
- **Bondlengths**: the number of bondlengths that are statistically significant according to Jackknife analysis, which looks at the bondlengths.
- **Bondangles**: the number of bondangles that are statistically significant according to Jackknife analysis, which looks at the bondangles.
- **Planarities**: the number of planarities in the structure, which includes peptide planes, and aromatic and nucleotide rings. In Coot, this is shown with Tangerine.
- **Chirals**: the number of chiral volumes that are outliers, which looks at the chirals.

Model and Data FS

This page shows the results from the model-to-map FSC, which is calculated using the phenix.mtriage command. Please see the phenix.mtriage documentation for more details on the calculation performed in FSC. Table 3 from the reference is reproduced below.

Metric	Typical of the map used in the calculation	Purpose
CC_{mask}	Fraction of signal	Detection of signal
CC_{volume}	Map & Envelope mask with a Fourier radius	Fit of the atomic centers
CC_{peaks}	Peak 20 points with the highest values in the model-map	Fit of the atomic centers in the most well-defined parts of the model-map
CC_{peaks}	Peak 20 points with the highest values in the model and in the map separately	Fit of the strongest peaks in the model and in the map
CC_{box}	Unmasked, cubic box with a Fourier radius	Fit of the atomic images in the cubic box of the model

Correlation coefficients per chain and per residue are also shown in plots.

Correlation plots

Correlation for A Correlation for B Correlation for C Correlation for D Correlation for E Correlation for F Correlation for G Correlation for H Correlation for I Correlation for J

The pin cushion and a zoom for a single chain. To change the chain, you can click on the pan chain pin or use the chain drop down. Clicking on the pin will change the center of the window in Coot.

Data

This page shows the output from phenix.mtriage. The output is the same as if one ran phenix.mtriage from the command line. Please see the phenix.mtriage documentation for more details.

The results are subdivided into several categories listed below.

- **Summary**: the phenix.mtriage statistics about the images and recommends the resolution estimates
- **FSC (Half-maps)**: this shows a graph plotting the Fourier shell coefficient curve based on the two half maps, as well as the recommended resolution based on the 0.143 cutoff.
- **FSC (Model-map)**: this shows a graph plotting the Fourier shell coefficient curve based on the full map and the model, as well as the recommended resolution based on the 0.143 cutoff.

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Multivalent, more and better reference data for improved all-atom structure validation. T.C. Terwilliger, P.V. Adams, R.O. Moriarty, M.L. Williams, R.M. Jakobi, R.M. Dyer, J.S. Lewis, D.A. Keedy, L.N. Kinch, J.M. Kriegler, M.L. Mayes, T.O. Yeates, W.A. Hendrickson, and D.L. Willis. P. Rosenzweig, Protein Science 30, 207-221 (2021). [Protein Science 30, 207-221 (2021)](https://doi.org/10.1002/pro.3987)

varref

Phenix *Python based Hierarchical Environment for Integrated Xtallography*

phenix.varref: a tool for refinement of a model against multiple data

Contents

- Description
- Availability
- Contact
- Command line examples
- Notes
- References

Description

phenix.varref, for 'variability refinement'. The program refines a model into an ensemble of maps derived from multiple datasets. The ensemble of maps represents the protein's heterogeneity captured during the experiment. The program can be used to refine a model against multiple datasets, for example datasets collected at several temperatures (ensemble) or multiplexed refinement (Wang et al. equivalent). The input of refinement with phenix.varref is a PDB file and a set of reflection files. The output is a multi-model PDB file and a series of maps. For more details refer to: http://dx.doi.org/10.1107/S2059798321.001170

Availability

phenix.varref is available in the command line and in the GUI.

Contact

For questions, bug reports, feature requests: help@phenix.lbl.gov

IMPORTANT: any problem report should be sent after trying the latest nightly build of Phenix:

http://cci.lbl.gov/cctbx_sources/phenix/nightly/build.zip

Please include the output of phenix.version in any bug report. Please also include the output of phenix.show_environment if it is not the version of Python that ships with the Phenix installation. It is very important that we know which version of Python we are using, and whether it is a standard installation or one that has been customized by us or one the Macintosh installation, which uses Anaconda Python rather than Macintosh Python.

Command line examples

1. A typical run:

```
phenix.varref model.pdb sigma=3 data1.mtz ... data2.mtz resolution=2.1
        output.prefix=test_varref
```

The program takes one model and list of maps in any order. The resolution is a mandatory parameter. Optional parameters include the output prefix, sigma (default is 3.0), the number of cycles (default is 5), the number of macro cycles (default is 3), the number of water cycles, and weight factor. Most of the keywords can be edited interactively, and are specified in the file varref.eff. The program also allows for refinement against multiple datasets, refinement against ensemble of models, refined against each individual map.

2. Refine ensemble with twenty models against

```
phenix.varref model.pdb sigma=3 data1.mtz ... data20.mtz \
        resolution=2.1 output.prefix=test_varref
```

Refinement against ensemble can be performed using RestraintLib of ecLIBM programs of Phenix and supplied to phenix.varref as an additional file.

3. Switching solvent, ligands and other small molecules to the macromolecule

```
phenix.varref model.pdb sigma=3 data1.mtz ... data20.mtz resolution=2.1
        output.prefix=test_varref
```

phenix.varref uses a better aggressive refinement strategies such as reseeding, simulated annealing, and weight optimization. The program also allows for refinement against multiple datasets, for example refinement against multiple datasets collected at different temperatures. Refinement against ensemble of models is possible using RestraintLib of ecLIBM programs of Phenix and supplied to phenix.varref as an additional file. Refinement against multiplexed data is also possible. The output of phenix.varref is a multi-model PDB file and a series of maps. The ensemble above this is done by providing a parameter file containing the following lines:

```
ensemble_refinement {
  ncycle = 5
  macro_ncycle = 1 stop if ave_cross_R_gap > 0
  water_ncycle = 1 stop if ave_cross_R_gap > 0 or ave_cross_R
  weight = 0.01 0.1 1.0
  ensemble_size = 20
  ignore_hydrogens = True
}
```

Once the varref output is chain X (chainid varchar 1) is linked to the Ensemble of residue ID's in chain B with the chain length of 20. The number of chains can be specified.

Notes

- The program can use multiple CPU. The program does use GPU. Running on single processor one ran one atom, one ran many CPU or cores.

References

- Wang Kai Cheng X, Minasyan L, Tworkowski L, Rosin M, Chandra V. Conformational space sampling in crystallographic refinement. Acta Crystallogr D Struct Biol. 2021 Jan 1;77(1):170-179. doi: 10.1107/S2059798321.001170. Epub 2021 Feb 5. PMID: 33475679.

PhenoMe *Python based Bioinstrument Microscopy for Integrated Multiscopy*

Structure factor file manipulations with Xmanip

Author(s)

- Andrew Martin Stuart
- Antonia Mey (Maintainer) Staff SE Scientific Computing

Purpose

Manipulation of reflection data and models

Uses

Command line interface

xmanip can be invoked via the command line interface with instructions given in a specific definition file. Usage is as follows:

The full set of definitions can be obtained by typing:

```
xmanip -help
```

```
which results in:

usage:
  xmanip [-i <file>]
  [-o <file>] [-log]
  [-mtzin <file>]
  [-mtzout <file>]
  [-pdbin <file>]
  [-pdbout <file>]
  [-mtzin2 <file>]
  [-mtzin3 <file>]
  [-mtzin4 <file>]
  [-stdin]
  [-stdout]
  [-rlim <lim> <lim>]

Program: 1.0
Author: Andrew Martin Stuart, pdb manipulation, utilities
Last update: 1 Sept 2010
  Usage: Input <file> [<label>] [<filter>], [<filter>] <out_pdb>[<out_mtz>]
  Input <file>[<label>] [<filter>]
```

Phenix

Afterscan Reactive Mutation to Acquire Antigenity

Data quality assessment with phenix.xtriage

Contents

- Authors
- Purpose
- Usage
- How xtriage works
- Output files from xtriage
- Xtriage keywords in detail
- Interpreting Xtriage output
- Twinning
- Anomalous signal
- Molecular weight
- Data preparation
- Sample histories
- Troubleshooting and problems
- Glossary
- Additional resources
- List of all available keywords

Authors

- Peter Zwart
- Ashley Deacon/Jeff Headd

Purpose

Phenix.xtriage is a tool for analyzing structure factor data to identify outliers, presence of twinning and other conditions that may cause structure to queer ?

Usage

How xtriage works

Most sanity checks performed by xtriage are:

- Wilson statistics
- Anomalous Wilson statistics
- Patterson analysis
- Ice ring analysis
- Twinning analysis
- Molecular weight estimation (possible in indexing: optional)
- Reflection statistics (completeness, redundancy, I/sigma)

See also: phenix.reflection_statistics, phenix.statistics.mtz (comparison of multiple data sets)

Output files from xtriage

- 1.*.log the log file contains all the screen output plus some cryst clash graphs
- 2.*.mtz the mtz file contains the scaled data
- 3.*.sca the scalepack file contains the scaled data

Xtriage keywords in detail

Scope: parameters.xtriage_scaling

```
data = "./data/*.sca" or "./data/*.mtz" or "./data/*.hkl"
  xtriage_output_directory = "./data/xtriage_output"
  scaling.input.xray_data.obs = "/data/data.sca"
```

These keywords are the minimum required input for the xtriage scale. If the number of residues/bases is not specified, a default condition of 300 is assumed.

Scope: parameters.hkl_data_parameters.xtriage_symmetry

```
  symmetry = "/data/data.pdb" or "/data/data.cif"
  unit_cell = 100.0 200.0 300.0 90.0 90.0 90.0
  space_group = "P 1 2 1" or "P 2 2 2" or "P 4 2 2" or "P 6 2 2"
```

The space group and unit cell keywords are optional if symmetry is considered to be flat enough to be considered a longer symmetry operator. Not both, space-as-space corresponds to the reflection count of the space group, and the unit cell keyword is used to calculate resolution. Although if there is no symmetry, neither unit cell nor SG will should be also.

Scope: parameters.hkl_data_parameters.xtriage_with_ncs

```
  ncs_group_1 = "/data/data.ncs" or "/data/data.pdb"
  ncs_group_2 = "/data/data.ncs" or "/data/data.pdb"
  ncs_group_3 = "/data/data.ncs" or "/data/data.pdb"
```

Phenix.xtriage can also take NCS operators into account. In a Trial Xtriage this determination of the twin fraction while taking into account NCS proves to be too tedious.

Scope: parameters.hkl_data_parameters.xtriage_with_ncs

```
  ncs_group_1 = "/data/data.ncs" or "/data/data.pdb"
  ncs_group_2 = "/data/data.ncs" or "/data/data.pdb"
  ncs_group_3 = "/data/data.ncs" or "/data/data.pdb"
  ncs_operators_are_identity_operators = yes
  ncs_operators_are_identity_operators = no
```

The possible determination of the resolution limit for the twinning test is determined on the basis of the ncs-corrected intensities. Although the ncs-corrected intensities are used for the twin test, the data used for the actual determination of the twinning fraction will be calculated by applications of the ncs operators. The default behavior is to assume the ncs operators are identity.

Scope: parameters.twinning

```
  twin = twinning = twinning_test
  twin_law = "h,-h-k,-l" or "-h-k,k,-l" or "h,k,-l"
  twin_fraction = 0.45 or 0.25 or 0.35
  twinning_test_resolution = 2.5
  twinning_test_resolution_ncs_corrected = 2.5
  twinning_test_resolution_ncs_corrected_for_twin_fraction = yes
  twinning_test_resolution_ncs_corrected_for_twin_fraction = no
```

Note that the twinning of specified and absent twin models is not doing matching algorithms.

Scope: scaling

```
  scaling.input.xray_data.obs = "/data/data.sca"
  scaling.input.xray_data.obs_lower = 0.0
  scaling.input.xray_data.obs_upper = 1.0
  scaling.input.xray_data.sigma_cutoff = 3.0
  scaling.input.xray_data.r_free_flags.ignore_all_zeros = true
  scaling.input.xray_data.r_free_flags.generate = true
  scaling.input.xray_data.r_free_flags.fraction = 0.10
  scaling.input.xray_data.r_free_flags.lattice_symmetry = hkl:p6/mmm
  scaling.input.xray_data.r_free_flags.n_bins = 20
  scaling.input.xray_data.r_free_flags.n_bins = 10
```

The scaling keywords are optional. These options are the well-suspected pattern removal. The data is cut around and the specified fraction of data. These options can be presented based upon the .sca or .mtz or .hkl. Although the .sca and .mtz are the preferred formats, the scaling keywords cannot be "lower-cut" and upper-cut scaled.

Interpreting Xtriage output

Twinny

```
  twinning_test_resolution_ncs_corrected_for_twin_fraction_yes_no
```

results in the following output (partial listing)

Matthews coeffs

```
  ------------------------------------------------------------------------
  ------------------------------------------------------------------------
  ------------------------------------------------------------------------
```

The Wilcoxon test is related to the monotonic trend test discussed above. Rar, also is the observed cumulative distribution of monotonic statistics of the current data, and uses the full distribution rather than just a p-value.

The effects of removing stones tend to flow into having a more sigmoidal character. In the case of pseudo-replication, the data will tend towards the flat.

Warning: Rar

This is a re-implementation developed by Sedlmeier and Gaskins (Ecol Lett (2005) 8:500-510) and is based on the original code by Sedlmeier. Unlike the original implementation, this version does not use a pre-calculated approximation, Wilcoxon's original and the Kendall tau statistic. A significant deviation of both tests tend to flag the expected values towards binomial or other problems.

```
Rar(x, y, ...)
  using Wilcoxon version, Rho,Rar of the form
  Rar(x, y, ...)
  where x, y are a pair of paired ranked vectors such that
  length(x) == length(y)
  Rho, Rar, Rho.p, Rho.n, Rho.p.adjust, Rho.n.adjust
  Rho.p.adjust.n, Rho.n.adjust.n, Rho.p.adjust.n.adjust
  The Kendall tau is returned whether it tests positive or
  negative correlation, the Wilcoxon tests are for positive
  correlation only, the .n versions are for negative tests.
```

Whether or not the data set is or is not a time series, the expected values, as shown in the first summary table below:

```
Rho.p.adjust.n  Rho.n.adjust.n  Rho.p.adjust.n.adjust
```

have two specific tests (Wilcox, 4 and Kendall, see below).

```
  Results of the Kendall and Wilcoxon tests
  Only 30.0% of the compared test pairs are used
  Rho.p.adjust.n: 0.00 corresponds to 100.00% Kendall
  Rho.n.adjust.n: 0.00 corresponds to 100.00% Kendall
  Rho.p.adjust.n.adjust: 0.00 corresponds to 100.00%
  Proportion of test failures is 100.00% (0.00 of 30.00)

  Wilcoxon versus
  Kendall tau-b estimate is 0.00 (-1.00, 1.00)
  Wilcoxon p.adjusted is 0.00
  Kendall p.adjusted is 0.00

  P.A.Sedlmeier's
  Rar(x, y, ...) Rho.p.adjusted: (NAN) NAN, 0/0
  Rho.p.adjusted NAN, 0.00
  Rho.n.adjusted NAN, 0.00
  Rho.p.adjusted.n 0.00
  Rho.n.adjusted.n 0.00
  Rho.p.adjusted.n.adjusted 0.00
  Rho.n.adjusted.n.adjusted 0.00
```

Revised Wilcoxon test from Sedlmeier/Gaskins
  Part, Rho, Rho.p.adjusted, Rho.n.adjusted
  Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n

These tests are based on the Wilcoxon test and are of calculated data is assumed, determine if statistical people according to present another better (Kendall tau) computational equivalency. It is estimated the Wilcoxon test is a good approximation to the Kendall tau test, and the Wilcoxon test is the one that is the commonly used.

```
  Results of the Kendall tau-b and Wilcoxon tests
  Kendall tau-b estimate is 0.00 (-1.00, 1.00)
  Wilcoxon p.adjusted is 0.00
  Kendall p.adjusted is 0.00
  P.A.Sedlmeier's Rho.p.adjusted: (NAN) NAN, 0/0
  Rho.p.adjusted NAN, 0.00
  Rho.n.adjusted NAN, 0.00
  Rho.p.adjusted.n 0.00
  Rho.n.adjusted.n 0.00
  Rho.p.adjusted.n.adjusted 0.00
  Rho.n.adjusted.n.adjusted 0.00
  Revised Wilcoxon test from Sedlmeier/Gaskins
    Part, Rho, Rho.p.adjusted, Rho.n.adjusted
    Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n
```

These tests are based on the Wilcoxon test and are of calculated data is assumed, determine if statistical people according to present another better (Kendall tau) computational equivalency. It is estimated the Wilcoxon test is a good approximation to the Kendall tau test, and the Wilcoxon test is the one that is the commonly used.

```
  Results of the Kendall tau-b and Wilcoxon tests
  Kendall tau-b estimate is 0.00 (-1.00, 1.00)
  Wilcoxon p.adjusted is 0.00
  Kendall p.adjusted is 0.00
  P.A.Sedlmeier's Rho.p.adjusted: (NAN) NAN, 0/0
  Rho.p.adjusted NAN, 0.00
  Rho.n.adjusted NAN, 0.00
  Rho.p.adjusted.n 0.00
  Rho.n.adjusted.n 0.00
  Rho.p.adjusted.n.adjusted 0.00
  Rho.n.adjusted.n.adjusted 0.00
  Revised Wilcoxon test from Sedlmeier/Gaskins
    Part, Rho, Rho.p.adjusted, Rho.n.adjusted
    Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n
```

The data frame obtained by this method is usually lower than what is obtained by refinement. The estimated proportion of failures, summarized, the possible space proper are listed as well (non-stress tests).

Run pairwise summary:

The results of the tests pairwise are summarized. Typical output looks as follows for cases of wrong symmetry, non-linear, non-monotonic trending and normal data hypothesis.

Wrong symmetry:

```
  Testing and linearity statistics summary (sample) data:
  Statistic comparison of test tau
    Kendall tau-b 0.00
    Wilcoxon p.adj 0.00
    Kendall p.adj 0.00
    Rho.p.adjusted NAN
    Rho.n.adjusted NAN
    Rho.p.adjusted.n 0.00
    Rho.n.adjusted.n 0.00
    Rho.p.adjusted.n.adjusted 0.00
    Rho.n.adjusted.n.adjusted 0.00
    Proportion of test failures 100.00% (0.00 of 30.00)
    Proportion of test pairs used 30.00%
    Rho.p.adjusted.n: 0.00 corresponds to 100.00% Kendall
    Rho.n.adjusted.n: 0.00 corresponds to 100.00% Kendall
    Rho.p.adjusted.n.adjusted: 0.00 corresponds to 100.00%
    Rho.n.adjusted.n.adjusted: 0.00 corresponds to 100.00%
    Revised Wilcoxon test from Sedlmeier/Gaskins
      Part, Rho, Rho.p.adjusted, Rho.n.adjusted
      Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n
    Rho.p.adjusted.n.adjusted 0.00
    Rho.n.adjusted.n.adjusted 0.00
    Revised Wilcoxon test from Sedlmeier/Gaskins
      Part, Rho, Rho.p.adjusted, Rho.n.adjusted
      Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n
```

Non-linear:

```
  Testing and linearity statistics summary (sample) data:
  Statistic comparison of test tau
    Kendall tau-b 0.00
    Wilcoxon p.adj 0.00
    Kendall p.adj 0.00
    Rho.p.adjusted NAN
    Rho.n.adjusted NAN
    Rho.p.adjusted.n 0.00
    Rho.n.adjusted.n 0.00
    Rho.p.adjusted.n.adjusted 0.00
    Rho.n.adjusted.n.adjusted 0.00
    Proportion of test failures 100.00% (0.00 of 30.00)
    Proportion of test pairs used 30.00%
    Rho.p.adjusted.n: 0.00 corresponds to 100.00% Kendall
    Rho.n.adjusted.n: 0.00 corresponds to 100.00% Kendall
    Rho.p.adjusted.n.adjusted: 0.00 corresponds to 100.00%
    Rho.n.adjusted.n.adjusted: 0.00 corresponds to 100.00%
    Revised Wilcoxon test from Sedlmeier/Gaskins
      Part, Rho, Rho.p.adjusted, Rho.n.adjusted
      Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n
    Rho.p.adjusted.n.adjusted 0.00
    Rho.n.adjusted.n.adjusted 0.00
    Revised Wilcoxon test from Sedlmeier/Gaskins
      Part, Rho, Rho.p.adjusted, Rho.n.adjusted
      Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n
```

Non-monotonic trending:

```
  Testing and linearity statistics summary (sample) data:
  Statistic comparison of test tau
    Kendall tau-b 0.00
    Wilcoxon p.adj 0.00
    Kendall p.adj 0.00
    Rho.p.adjusted NAN
    Rho.n.adjusted NAN
    Rho.p.adjusted.n 0.00
    Rho.n.adjusted.n 0.00
    Rho.p.adjusted.n.adjusted 0.00
    Rho.n.adjusted.n.adjusted 0.00
    Proportion of test failures 100.00% (0.00 of 30.00)
    Proportion of test pairs used 30.00%
    Rho.p.adjusted.n: 0.00 corresponds to 100.00% Kendall
    Rho.n.adjusted.n: 0.00 corresponds to 100.00% Kendall
    Rho.p.adjusted.n.adjusted: 0.00 corresponds to 100.00%
    Rho.n.adjusted.n.adjusted: 0.00 corresponds to 100.00%
    Revised Wilcoxon test from Sedlmeier/Gaskins
      Part, Rho, Rho.p.adjusted, Rho.n.adjusted
      Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n
    Rho.p.adjusted.n.adjusted 0.00
    Rho.n.adjusted.n.adjusted 0.00
    Revised Wilcoxon test from Sedlmeier/Gaskins
      Part, Rho, Rho.p.adjusted, Rho.n.adjusted
      Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n
```

Normal data:

```
  Testing and linearity statistics summary (sample) data:
  Statistic comparison of test tau
    Kendall tau-b 0.00
    Wilcoxon p.adj 0.00
    Kendall p.adj 0.00
    Rho.p.adjusted NAN
    Rho.n.adjusted NAN
    Rho.p.adjusted.n 0.00
    Rho.n.adjusted.n 0.00
    Rho.p.adjusted.n.adjusted 0.00
    Rho.n.adjusted.n.adjusted 0.00
    Proportion of test failures 100.00% (0.00 of 30.00)
    Proportion of test pairs used 30.00%
    Rho.p.adjusted.n: 0.00 corresponds to 100.00% Kendall
    Rho.n.adjusted.n: 0.00 corresponds to 100.00% Kendall
    Rho.p.adjusted.n.adjusted: 0.00 corresponds to 100.00%
    Rho.n.adjusted.n.adjusted: 0.00 corresponds to 100.00%
    Revised Wilcoxon test from Sedlmeier/Gaskins
      Part, Rho, Rho.p.adjusted, Rho.n.adjusted
      Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n
    Rho.p.adjusted.n.adjusted 0.00
    Rho.n.adjusted.n.adjusted 0.00
    Revised Wilcoxon test from Sedlmeier/Gaskins
      Part, Rho, Rho.p.adjusted, Rho.n.adjusted
      Rho.p.adjusted.n.adjusted, Rho.n.adjusted.n
```

In the summary, the significance of the deviation of the values of the t-test from normality are stated. The Kendall tau-b and the Wilcoxon tau are the statistics commonly used for the procedure.

Examples

Standard use of sitrace

Running sitrace is easy. From the command line you can type:

```
sitrace.sitrage data.csv
```

When an RCS or CSV file is used, sitrace tests to be specified:

```
sitrace.sitrage -t "Kendall,Wilcoxon,Rho,Rho.p.adjusted,Rho.n.adjusted" -f "Rho.p.adjusted.n.adjusted" -l -r -s -v -w -x -y data.csv
```

In order to perform a Wilcoxon test, sitrace. It might be useful to specify the number of workers/threads in the (multithread mapcc module).

```
sitrace.sitrage -t "Wilcoxon" -w 4 -l -r -s -v -x -y -f "Rho.p.adjusted.n.adjusted" -t "Wilcoxon" -w 4 data.csv
```

By default the sitrace-sitrage uses additional (call-step) graphs (viewable with the (call-progress-logger) and activate is the normal logfile log. The (nonlinear) line (dynamic) and all other default settings are summarized in the (sitrace-sitrage -h) help guide (or frequency plotting (-l) linear values).

```
sitrace.sitrage [-]
  [-h|--help|-?]
  [-v|--verbose]
  [-l|--log|--log-file]
  [-r|--rho|--rho-test]
  [-s|--sort|--sort-data]
  [-x|--x-axis|--x-axis-data]
  [-y|--y-axis|--y-axis-data]
  [-t|--test|--test-data]
    "Kendall,Wilcoxon,Rho,
    Rho.p.adjusted,Rho.n.adjusted,
    Rho.p.adjusted.n,Rho.n.adjusted.n,
    Rho.p.adjusted.n.adjusted,Rho.n.adjusted.n.adjusted"
  [-f|--filter|--filter-data]
    "Rho.p.adjusted.n.adjusted"
  [-w|--workers|--threads]
    4
  [-d|--dynamic|--dynamic-data]
  [-n|--nonlinear|--nonlinear-data]
  [-m|--monotonic|--monotonic-data]
  [-p|--progress|--progress-data]
  [-c|--call-step|--call-step-data]
  [-e|--error|--error-data]
  [-a|--all|--all-data]
  [-o|--output|--output-data]
    "data.csv"
  [-i|--input|--input-data]
    "data.csv"
  [-g|--graph|--graph-data]
    "data.csv"
  [-b|--binary|--binary-data]
    "data.csv"
  [-u|--usage|--usage-data]
    "data.csv"
  [-q|--quiet|--quiet-data]
    "data.csv"
  [-k|--kill|--kill-data]
    "data.csv"
  [-j|--jobs|--jobs-data]
    "data.csv"
  [-z|--zero|--zero-data]
    "data.csv"
  [-w|--workers|--threads]
    4
  [-d|--dynamic|--dynamic-data]
  [-n|--nonlinear|--nonlinear-data]
  [-m|--monotonic|--monotonic-data]
  [-p|--progress|--progress-data]
  [-c|--call-step|--call-step-data]
  [-e|--error|--error-data]
  [-a|--all|--all-data]
  [-o|--output|--output-data]
    "data.csv"
  [-i|--input|--input-data]
    "data.csv"
  [-g|--graph|--graph-data]
    "data.csv"
  [-b|--binary|--binary-data]
    "data.csv"
  [-u|--usage|--usage-data]
    "data.csv"
  [-q|--quiet|--quiet-data]
    "data.csv"
  [-k|--kill|--kill-data]
    "data.csv"
  [-j|--jobs|--jobs-data]
    "data.csv"
  [-z|--zero|--zero-data]
    "data.csv"
```

The defaults are good for most applications.

Possible Problems

Specific limitations and problems

- Average doesn't deal with data in series (space groups

Literature

- CCPs newsletter No. 41, Summer 2005: Characterization of X-ray data sets
- Sedlmeier and Gaskins (Ecol Lett (2005) 8:500-510) Robust statistical assessment of X-ray data sets and extensions Wilcoxon Rho calculation

Additional information

List of all available keywords

```
sitrage
  [-h|--help|-?]
    [-v|--verbose]
    [-l|--log|--log-file]
    [-r|--rho|--rho-test]
    [-s|--sort|--sort-data]
    [-x|--x-axis|--x-axis-data]
    [-y|--y-axis|--y-axis-data]
    [-t|--test|--test-data]
      "Kendall,Wilcoxon,Rho,
      Rho.p.adjusted,Rho.n.adjusted,
      Rho.p.adjusted.n,Rho.n.adjusted.n,
      Rho.p.adjusted.n.adjusted,Rho.n.adjusted.n.adjusted"
    [-f|--filter|--filter-data]
      "Rho.p.adjusted.n.adjusted"
    [-w|--workers|--threads]
      4
    [-d|--dynamic|--dynamic-data]
    [-n|--nonlinear|--nonlinear-data]
    [-m|--monotonic|--monotonic-data]
    [-p|--progress|--progress-data]
    [-c|--call-step|--call-step-data]
    [-e|--error|--error-data]
    [-a|--all|--all-data]
    [-o|--output|--output-data]
      "data.csv"
    [-i|--input|--input-data]
      "data.csv"
    [-g|--graph|--graph-data]
      "data.csv"
    [-b|--binary|--binary-data]
      "data.csv"
    [-u|--usage|--usage-data]
      "data.csv"
    [-q|--quiet|--quiet-data]
      "data.csv"
    [-k|--kill|--kill-data]
      "data.csv"
    [-j|--jobs|--jobs-data]
      "data.csv"
    [-z|--zero|--zero-data]
      "data.csv"
    [-w|--workers|--threads]
      4
    [-d|--dynamic|--dynamic-data]
    [-n|--nonlinear|--nonlinear-data]
    [-m|--monotonic|--monotonic-data]
    [-p|--progress|--progress-data]
    [-c|--call-step|--call-step-data]
    [-e|--error|--error-data]
    [-a|--all|--all-data]
    [-o|--output|--output-data]
      "data.csv"
    [-i|--input|--input-data]
      "data.csv"
    [-g|--graph|--graph-data]
      "data.csv"
    [-b|--binary|--binary-data]
      "data.csv"
    [-u|--usage|--usage-data]
      "data.csv"
    [-q|--quiet|--quiet-data]
      "data.csv"
    [-k|--kill|--kill-data]
      "data.csv"
    [-j|--jobs|--jobs-data]
      "data.csv"
    [-z|--zero|--zero-data]
      "data.csv"
  [-h|--help|-?]
    Help message
  [-v|--verbose]
    Verbose output
  [-l|--log|--log-file]
    Log file
  [-r|--rho|--rho-test]
    Rho test
  [-s|--sort|--sort-data]
    Sort data
  [-x|--x-axis|--x-axis-data]
    X-axis data
  [-y|--y-axis|--y-axis-data]
    Y-axis data
  [-t|--test|--test-data]
    Test data
    "Kendall,Wilcoxon,Rho,
    Rho.p.adjusted,Rho.n.adjusted,
    Rho.p.adjusted.n,Rho.n.adjusted.n,
    Rho.p.adjusted.n.adjusted,Rho.n.adjusted.n.adjusted"
  [-f|--filter|--filter-data]
    Filter data
    "Rho.p.adjusted.n.adjusted"
  [-w|--workers|--threads]
    Workers/threads
    4
  [-d|--dynamic|--dynamic-data]
    Dynamic data
  [-n|--nonlinear|--nonlinear-data]
    Nonlinear data
  [-m|--monotonic|--monotonic-data]
    Monotonic data
  [-p|--progress|--progress-data]
    Progress data
  [-c|--call-step|--call-step-data]
    Call step data
  [-e|--error|--error-data]
    Error data
  [-a|--all|--all-data]
    All data
  [-o|--output|--output-data]
    Output data
    "data.csv"
  [-i|--input|--input-data]
    Input data
    "data.csv"
  [-g|--graph|--graph-data]
    Graph data
    "data.csv"
  [-b|--binary|--binary-data]
    Binary data
    "data.csv"
  [-u|--usage|--usage-data]
    Usage data
    "data.csv"
  [-q|--quiet|--quiet-data]
    Quiet data
    "data.csv"
  [-k|--kill|--kill-data]
    Kill data
    "data.csv"
  [-j|--jobs|--jobs-data]
    Jobs data
    "data.csv"
  [-z|--zero|--zero-data]
    Zero data
    "data.csv
```

xtriage_gui

Phenix *Python based Hierarchical Environment for Integrated Xtallography*

The phenix.xtriage graphical interface

Contents:

- Video Tutorial
- Introduction
- Interpreting Xtriage output
  - Alerts for problematic results
  - Interpreting statistics
  - Data quality assessment
  - Twinning and pseudo-translational analysis, Wilson plots
  - Ice ring detection
  - Anomalous signal
- Merging statistics
  - Merging statistics
  - Data quality assessment, Wilson statistics
  - Twin law detection

Video Tutorial:

The basic Xtriage tutorial video is available on the Phenix YouTube channel and explains how to run phenix.xtriage from the GUI.

The advanced Xtriage tutorial (1 hr) covers the ice ring analysis (the video starts on the tutorial chapter):

- Introduction
- Translational NCS (10m)
- Twinning
- Wilson plot and pseudo-translation, ice rings & Wilson (15m)

Configuration

Since the phenix.xtriage output is a reference file and summary information, (and the MTZ files is automatically checked), it seems to be the Phenix-GUI wrapping expected output (which is made the GUI or directly if phenix.xtriage is run from the command line).

To launch Xtriage, open the menu Macro-Ext and click on or drag and drop a reflection file into the Xtriage window. Then, select some data and the Xtriage configuration dialog will appear, recognizing the command line options. Also, which data are used, the output directory and a prefix can be specified.

The **Parameters** button opens a window containing the most essential information about the reflection data, such as the number of reflections, the resolution range, the space group, the unit cell parameters, and the wavelength. The Xtriage tab lists Xtriage and Xtriangle options, and analogously, the **Advanced** of MTZ data **Advanced** GUI. In the Xtriage tab, the **Xtriangle** button allows to run Xtriangle, which is a tool for the analysis of Wilson plots and ice rings. Only that tool does not output reflections and requires at minimum only the input data and a prefix. Xtriangle is a tool for the analysis of Wilson plots and ice rings. Xtriangle is a tool for the analysis of Wilson plots and ice rings. Xtriangle is a tool for the analysis of Wilson plots and ice rings

Data quality analyses

Data quality analyses are important and of great to many data, converted with data by repository design, and of data quality design to design to design to design to design. Data quality analyses are based on the stages of data quality design to design to design to design to design. Data quality analyses are based on the stages of data quality design to design to design to design to design. Data quality analyses are based on the stages of data quality design to design to design to design to design. Data quality analyses are based on the stages of data quality design to design to design to design to design.

Completeness and dos strength

The following table lists the completeness in various resolution ranges, after applying to map up. After binning the data into resolution shells, the completeness is calculated for each shell. The last shell is the overall completeness of the dataset. The binning completeness profile is an indicator of the strength of the data.

The following table lists the completeness in various resolution ranges, after applying to map up. After binning the data into resolution shells, the completeness is calculated for each shell. The last shell is the overall completeness of the dataset.

Fitting for Offset
Fitting for Offset
Fitting for Offset