aRMSD-primer (aRMSD 0.9.8)

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The goal of the primer is to enable you to perform a basic comparison of two molecular structures with `aRMSD`, including proper installation of the program. Here and there, the primer merely will *hint* you to additional features implemented in `aRMSD`.

1 setup of `aRMSD`

Initially, Arne Wagner developed `aRMSD` under Windows. Hence, the corresponding section below retains all the relevant recommendations by him as left in 2017 in the original branch of the project of `aRMSD`. The copy is verbatim, with the exception of putting the information into one place, a reformat, and a spell check. As outlined in branch `compilerIssueWindows`, however, it is possible that the original script `compile_aRMSD.py` does not work. If so, either checkout branch `compilerIssueWindows` with an updated compiler script (different name), or use a setup in Linux Debian (testing) as outlined below.

This forked branch is based on the original version 0.9.6 by Arne Wagner. It was developed further in Debian 10 (Sid/buster) because `aRMSD` was used side-by-side with other programs already deployed successfully in Linux. The installation process differs from the one in Windows, as `pip` and `PyInstaller` are omitted, and the installation of dependencies is automated by a script.

1.1 setup in Windows, outlined by Arne Wagner

`aRMSD` can be in two ways, either via `pip` (in this case it will be used as a Python module or Python application) or you can download the source code and compile it into a single standalone executable. In any case some packages are required which are listed below:

- `Python` (version 2.7 or 3.6)
- `numpy` (version 1.11.1 / 1.12)
- `vtk` (version 6.2.0 / 7.0)
- `matplotlib` (version 1.5.2 / 2.0)
- `PyQt4`

- uncertainties (version 3.0.1)

optional:

- Cython [performance improvements] (version 0.25.2)
- openbabel / pybel [additional file formats] (version 2.4.1)

Due to changes from vtk 5 to 6, aRMSD does not support an older vtk version than 6.2 and a backwards compatibility to the older vtk 5 engine is not planned.

In order to adjust the source code by yourself, always make sure to have the required Python packages installed and download the latest version of the master branch. Whenever possible it is recommended to add and update packages using pre-compiled Python wheels (http://www.lfd.uci.edu/~gohlke/pythonlibs/) suited for your operating system which can be installed via pip.

1.1.1 Compilation arguments

The following arguments can be passed to the installation script and specify the usage of Cython and openbabel in the compilation. All arguments are optional and if none are given neither Cython nor openbabel will be used. The specification of the C compiler may not be needed if your defaults are properly set, however setting it explicitly should ensure a successful installation.

- --use_cython (True / False)
- --cython_compiler (any valid C compiler used by Cython, e.g. msvc)
- --use_openbabel (True / False)
- --overwrite (True / False)

During the installation, the existence of an openbabel hook file in the PyInstaller hook path is checked. If no hook exists, a respective file will be created. In case of an existing hook, the file can be overwritten if the --overwrite variable is set to True.

1.1.2 Executable compiled with PyInstaller

This produces a single file which can be copied alongside the settings.cfg and the xsf folder to different machines with the same architecture. Once the program has been compiled, this is probably the easiest way to use aRMSD – especially for users that are unfamiliar with Python.

First ensure that you have the latest version of PyInstaller (http://www.pyinstaller.org/) or install it with pip:

```
pip install pyinstaller
```

Download the current master branch of aRMSD, extract the files and navigate to the main folder. Run the compilation script in an interactive Python shell or from command line by typing

```
python compile_aRMSD.py
```

This will create a single executable file in the `armsd` folder and should work for all operating systems. Temporary files will be created during this process (the compilation will take around 30 min, depending on the machine) and deleted after the executable is created. Optional arguments can be given to make use of `Cython` (`http://cython.org/`) and `openbabel` (`http://openbabel.org/wiki/Main_Page`). Note that the `Cython C compiler` should be specified if several options are available:

```
python compile_aRMSD.py --use_cython=True --cython_compiler=msvc --use_openbabel=True
↪  --overwrite=True
```

If you are using Python 3.6, there is a bug in the `PyInstaller` entry script and typing `pyinstaller` in a shell will not start a correct process. To fix this, go in the Python installation folder and edit the `pyinstaller-script.py` file: add quotes around the path in the first program line (e.g. `"c:\program files\python36\python.exe"`).

1.1.3 comment on Arne Wagner's setup in Windows

In a recent test (December 2018), I was not able to replicate Arne Wagner's approach to set-up `aRMSD` in Windows as outlined above. However, and meant as a *temporary fix* only, `aRMSD` equally may be run within the portable `WinPython` system – then using Python (version 3.6.5) – amended by a suitable vtk-wheel in Windows 7 (64 bit). Details about this approach are provided on `https://github.com/nbehrnd/aRMSD-minimalWindowsSupport`.

2 Setup of aRMSD in Linux Debian / Ubuntu

In addition to the `*.zip` archive available on GitHub, `aRMSD` depends on libraries most likely not installed on your computer. Anticipate about 0.2 to 0.3 GB of disk space needed for them.

For a facile, semi-automatic set-up, the top directory of the extracted archive contains script `debcollector_aRMSD.py` which you shall run once from the CLI prior to any use of `aRMSD`:

```
python debcollector.py
```

This script is dedicated to the deployment under Linux Debian (e.g., Debian 9 (Sid/buster), or Xubuntu (Xubuntu 18.04 LTS). It will request the administrator password, and triggers the system to fetch and install the dependencies of `aRMSD` in one run. Possibly, user interaction is needed since this process may recursively install modules *in addition* to the ones explicitly listed in the script.

If you use a different operating system, or prefer a manual package installation, here are the relevant modules I use on a reference system (Debian 9, Sid/buster) to work with `aRMSD`:

- `python` (version 2.7.15+) and `python3` (version 3.6.6)
- `cython` (version 0.28.4-1)

- `openbabel`, `libopenbabel5`, `python-openbabel` (all in version 2.4.1+dfsg-2)
- `python-matplotlib`, `python-matplotlib-data`, `python3-matplotlib` (all in version 2.2.2-4+b1)
- `python-uncertainties`, `python3-uncertainties` (all in version 2.4.4-1)
- `libvtk6.3`, `libvtk6.3-qt`, `python-vtk6`, `vtk6` (all in version 6.3.0+dfsg2-2+b3); `libvtk7.1`, `libvtk7.1-qt`, `python3-vtk7`, `vtk7` (all in version 7.1.1+dfsg1-5)

Again, note that according to Arne Wagner's description about `aRMSD` running in Windows, you may skip `cython` wich will provide an *optional* gain in performance.

After completed installation of these dependencies, enter the top directory of the decompressed archive with your shell, and start `aRMSD`:

```
python armsd/aRMSD.py
```

The first start of the program is slower than the subsequent ones, but your terminal should display a welcome screen similar to the one in figure 1.

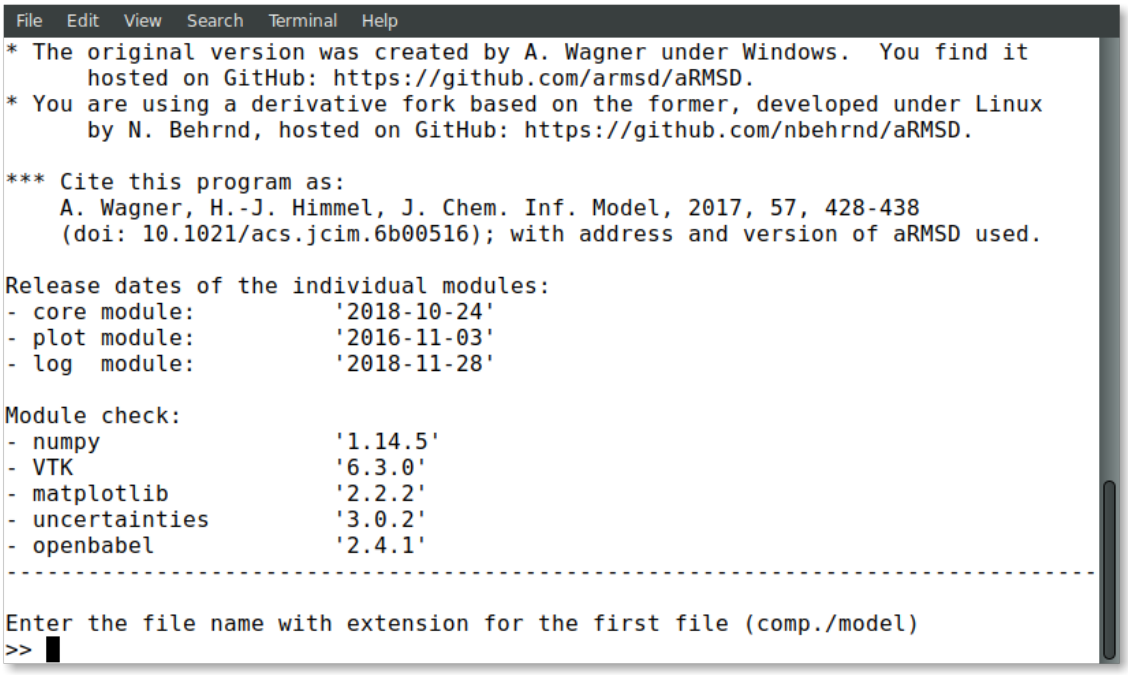

Figure 1: Initial screen display of `aRMSD` in a 80 × 24 character terminal.

While it is possible to work in the default dimension of a terminal with 80 × 24 characters, you may miss some of the intermediate output provided by `aRMSD` by omission of vertical scrolling.

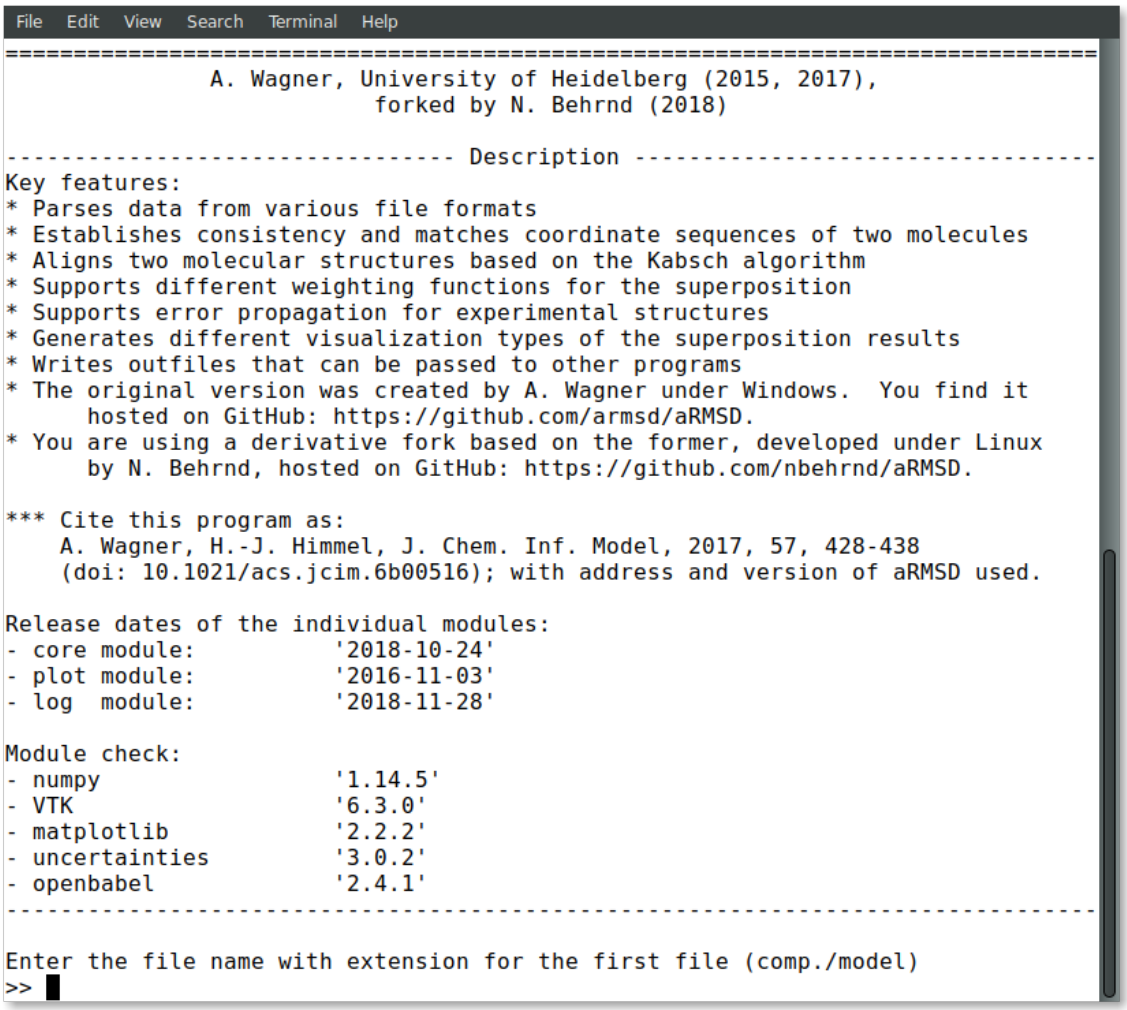

Figure 2: Initial screen display of aRMSD in a 80 × 43 character terminal.

Hence, a taller terminal is recommended, e.g., 80 × 43 characters, as shown in figure 2. However, a terminal wider than 80 characters per line will not provide additional benefit.

Like other python scripts run in the CLI, at any stage of working with aRMSD the program may be closed safely from the terminal with the command Ctrl + C.

The vtk related modules are *essential* to work with aRMSD. Still, it is possible to access a subset of functions provided by aRMSD with a few of the other modules modules missing. In particular, this is if

- your system does not spot libopenbabel. Then, file format conversions provided by babel will be unavailable to aRMSD. In this situation, the only model file type accessible to the program is *.xyz.
- your system lacks matplotlib. Then, there will be no provision of the 2D statistics plots. Since the corresponding sub-routine in aRMSD equally contributes some numerical results, the eventual log generated by aRMSD will miss portions of the diagnostic data.

In both cases the welcome screen will tell you about the modules missing / not recognized by the installation. Yet even in this situation aRMSD still will be capable to align the structure models, refine their alignment and provide you with some of the results of the similarity analysis. You are set to work with aRMSD.

3 Example comparing two models successfully

This chapter will detail out how to compare successfully to model data with the basic test data provided with aRMSD. It is complemented by the next section about how to identify an unsuccessful comparison of two model data. In addition, the complete CLI output by aRMSD as well as the log are provided in the corresponding section of the appendix.

In sub-folder examples, aRMSD provides a few test data to familiarize with the program. For the sake of simplicity, this tutorial will use model data in the most basic file format accessible for aRMSD – even if your system lacks babel – which is *.xyz. Copy the model data M1.xyz and M2.xyz into the folder armsd. These two represent two different conformations of the aspirinate anion, derived from the corresponding *.cif found in the CSD data base.[1] They were simplified to the aspirinate anion, retaining protons, and exported in either *.xyz or *.pdb format with Olex2.[2]

[1] Model M1.xyz and M1.pdb are derivated from entry FEHGAB, while M2.xyz and M2.pdb are derivated from entry IVUYEE of the Cambridge Crystallographic Data Base. The *primary* references for the model data are: FEHGAB / basis for model M1.xyz: "Five-coordinate nickel(II) complexes with carboxylate anions and derivatives of 1,5,9-triazacyclododec-1-ene: structural and 1H NMR spectroscopic studies" by M. D. Santana, A. A. Lozano, G. Garcia, G. Lopez, J. Perez, *Dalton Transactions*, 2005, 104–109 (doi: 10.1039/B413547D). And for IVUYEE, basis for model M2.xyz: "Synthesis, structural characterization and biological studies of novel mixed ligand Ag(I) complexes with triphenylphosphine and aspirin or salicylic acid" by M. Poyraz, C. N. Banti, N. Kourkoumelis, V. Dokorou, M. J. Manos, M. Simčič, S. Golič-Grdadolnik, T. Mavromoustakos, A. D. Giannoulis, I. I. Verginadis, K. Charalabopoulos, S. K. Hadjikakou, *Inorganica Chimica Acta*, 2011, *375*, 114–121 (doi: 10.5517/ccv2f3f).

[2] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H., OLEX2: A complete structure solution, refinement and analysis program (2009). *J. Appl. Cryst.*, 42, 339–341. Olex2, version 1.2.10.

- From the top directory of aRMSD, launch the program from the shell with

  ```
  python armsd/aRMSD.py
  ```

  After the simulated prompt (the > sign), enter the complete file name (including the file extension) of the first model to load. Contrary to the shell, there is no tab-assisted auto-completion of the file name. If you err with the file name, and the model does not exist, you are offered a new prompt. If you err with the file name pointing to an exisiting model, but are not interested to compare with an other model, the simplest rectification is to close aRMSD with `Ctrl + C` and to start the program freshly again.

  The confirmation of the input (`Enter`) will cause aRMSD to read the data set and to prompt you for the input of the second model datum (fig 3).

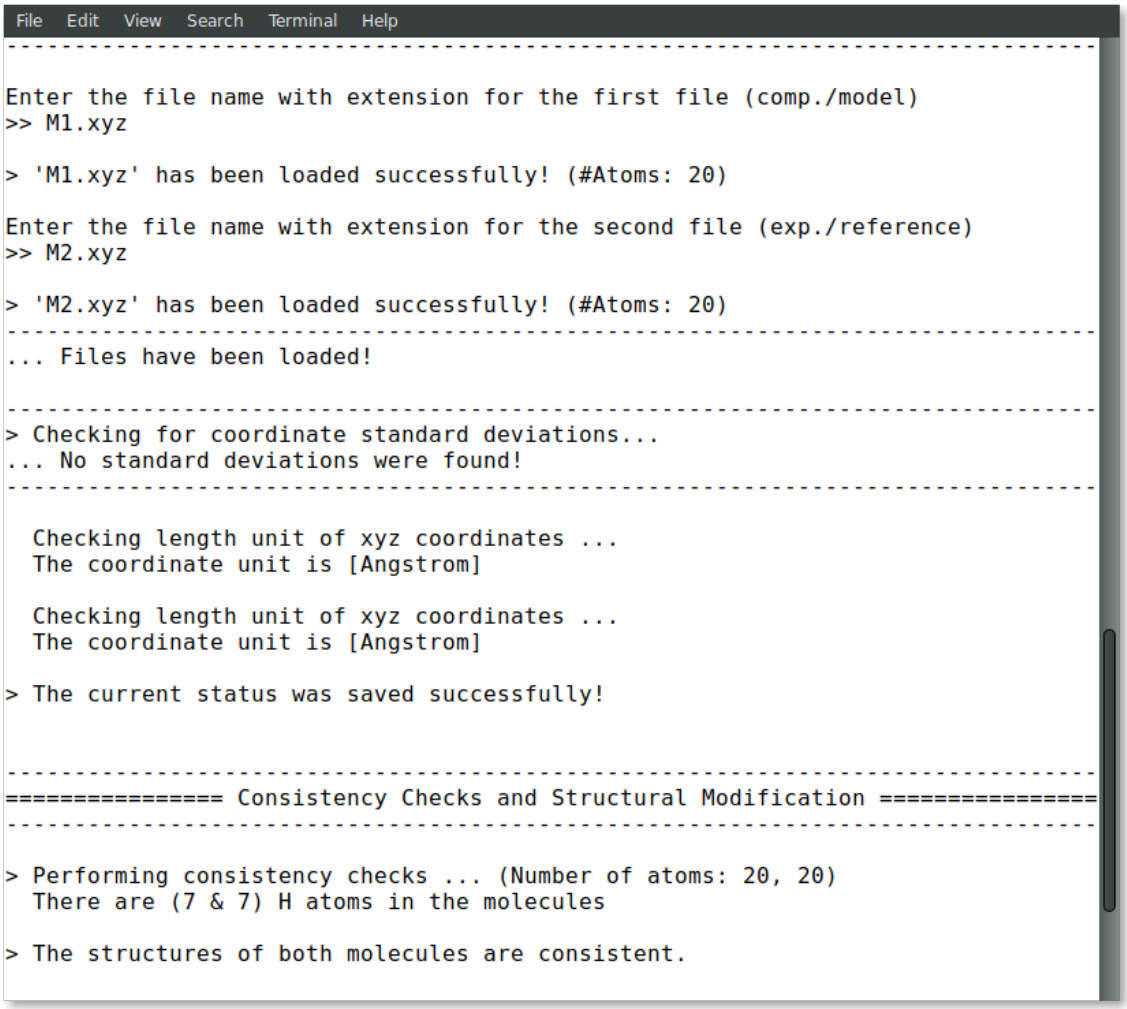

Figure 3: Model loading and consistency check by aRMSD.

The atom coordinates provided in either `*.xyz` (*this* example) or `*.pdb` format provide the the atom coordinates as a tuple of three numbers only. This contrasts to the `*.cif` format where the coordinates are provided including their standard deviations. So, `aRMSD` *indicates* the user about this information missing. Based on the file type of the model data, you may continue the analysis neglecting this.

Hint: Indeed, it is possible to load different models of different file type (with different file extensions), such as `M1.xyz` for the first, and `M2.pdb` for the second model to compare with each other. At this stage of the analysis, `aRMSD` will proceed successfully provided both models share the same molecular constitution. This is tested in the `Consistency Check` mentioned in the lower part of the depicted output.

- Consideration of hydrogen atoms

  `aRMSD` allows you to include all, or to exclude a selection of hydrogens (bond to carbons, or bond to group-14 elements), or to consider none of the hydrogens in the structure models from the Kabsch test. This is done without editing the underlying files you provided, but will affect simultaneously both structure "model" and structure "reference".

  Generally speaking, compared with the comparison of "complete models", the exclusion of hydrogens may (and indeed most often will) increase the similarity of the structures perceived by `aRMSD`, expressed by a lower overall-RMSD. If you know that the positions of the hydrogens in your model data are considerably less accurately determined then the one of the non-hydrogen atoms, then this may be good option to test.[3]

  For the purpose of this primer, however, all atoms were included in the scrutiny (fig 4), selected by key stroke `3`.

  Hint: Beside a yes-no decision about hydrogens, `aRMSD` equally offers multiple more refined approaches how atoms will be considered in the Kabsch test. These then scale the individual contribution of the atoms' position to the RMSD to the proton count, the atomic mass, or the scattering factor (for the more frequently used X-ray radiation wavelengths). This accounts for the determination of the atom coordinates of heavier atoms being more accurate than for the lighter ones by X-ray diffraction analysis, an approach considered as advanced use of `aRMSD`.

  The program subsequently provides you a first reasonable *guess* how to align the two models.

- User-assisted re-orientation of the models

  This is the first time `aRMSD` will launch the `vtk`-based structure visualizer in a window separate from the terminal, providing an interactive 3D rendering (fig. 5). You may change the position and size of this window freely. The depicted scene shows you *an initial* alignment of atom labeled model (red motif) and reference structure (green motif) in a reference coordinate system (blue).

[3] To account for the different data quality is right one motivation of `aRMSD` to load module `incertainties`, on one hand, and to access the standard derivations of the atom coordinates provided in the structure data (e.g., `*.cif`), on the other.

```
File  Edit  View  Search  Terminal  Help
--------------------------------------------------------------------------------

> Performing consistency checks ... (Number of atoms: 20, 20)
  There are (7 & 7) H atoms in the molecules

> The structures of both molecules are consistent.

--------------------------------------------------------------------------------
    What should happen to the remaining 7 H-atoms?
--------------------------------------------------------------------------------
    Info: The exclusion of H-atoms in RMSD calculations is recommended if
          they were not located and refined in the X-ray experiment
--------------------------------------------------------------------------------
0   ... remove all hydrogen atoms (7)
3   ... keep all hydrogen atoms
--------------------------------------------------------------------------------

>>  Enter your choice: 3

> The molecules were rotated into 'Standard Orientation' ...

> The current status was saved successfully!

--------------------------------------------------------------------------------
```

Figure 4: User defined exclusion / retention of hydrogens in aRMSD.

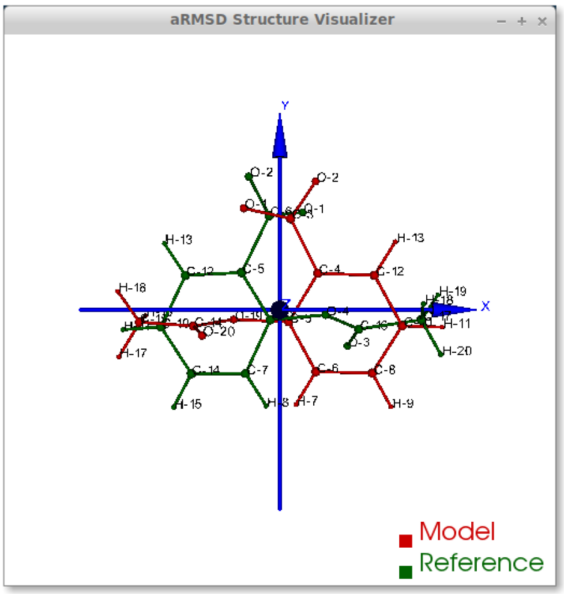

Figure 5: Vtk-based structure visualizer by aRMSD.

Multiple commands are at your disposition, outlined briefly in the table 1.

Table 1: Typical commands to interact with the structure visualizer in aRMSD.

command	function
dragging with left mouse button (LMB)	tilt the scene
CTRL + LMB	roll the scene
Shift + LMB	pane the scene
middle mouse reel	zoom the scene
r	return to a home position
3	toggle anaglyph display
e, or 0, or q	close the visualizer
s	save the scene (*.png)

Note that the more your mouse is out of the center of the visualizer's canvas, the more the mouse-assisted actions accelerate. You may document the match as bitmap with key-stroke s; the visualizer, unaltered in its default dimension will write a *.png (2048 × 2048 px). Repeated export of the scene, e.g., from different perspectives, will automatically increment the file names (VTK_initial_plot.png, VTK_initial_plot_1.png, VTK_initial_plot_2.png, etc.) deposit in your current working directory.

If you are familiar about the alignment shown to you, close the visualizer (q). If – as in the current example – the two model data do not align nicely, the terminal offers you multiple symmetry operations to try a better alignment (fig. 6). Each time you select one of the options, aRMSD displays a new *initial match* of the two in a newly opened instance of the visualizer.

In the case of this primer, the relative arrangement has to undergo an inversion (key-stroke 1), and an reflection in respect to the *xz*-plane (key-stroke 3). The approach is iterative, and the order of consecution of these operations does not matter. The progress is shown in figure 7. Intentionally both alignments shown share the same perspective.

At this stage, you aim for a fit of the two model structures that is *good enough*. (In the ongoing of this section, as well in comparison with the next chapter, you will learn what this refers to.) Once two structure data do overlap – again, it is *an initial* superposition only – close the visualizer (key-stroke q) and save this change alignment obtained (with key-stroke 10).

- Re-ordering of the atoms

  To proceed in the refinement of the superposition successfully, the atoms recognized of both models have to be labeled consistently. *One* approach available in aRMSD is the so-called Hungarian algorithm, implemented as default strategy. At the current stage of the analysis, this is triggered by hitting -1 (minus one).

  aRMSD will again open a vtk-visualizer of the two prealigned models (figure 8). In contrast to the former situation, however, the labeling of the atoms of one molecule should match

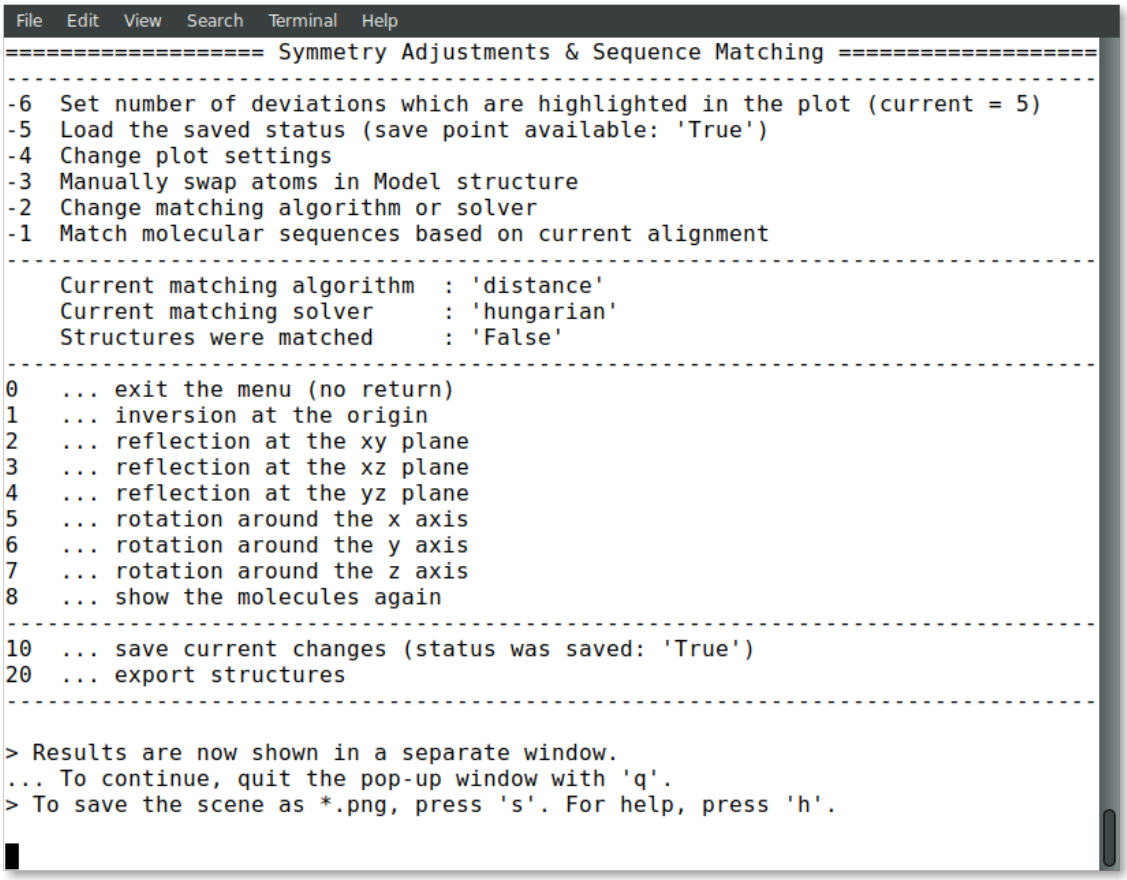

Figure 6: Symmetry operations provided by aRMSD to alter and improve the initial alignment of structure "model" and "reference".

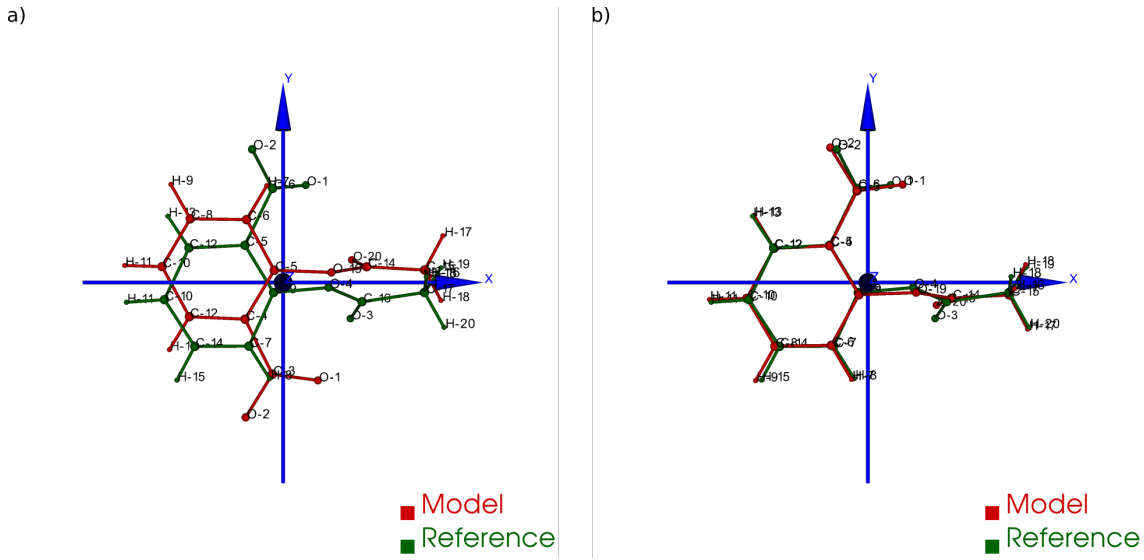

Figure 7: Example of progressively adjusting the relative alignment of structure "model" (`M1.xyz`) and "reference" (`M2.xyz`) in `aRMSD`. a) After application of an inversion. b) After subsequent application of inversion and reflection in respect to the *xz*-plane.

the one of the same atoms in the second molecule. In addition, yellow streaks will indicate which atoms with greater distance to each other `aRMSD` considers as equivalent.

Since the obtained match is reasonable, close the visualizer (key-stroke `q`), and save the intermediate result (key-stroke `10`).

- Refinement of the superposition and Kabsch test

  To enter the menu about the Kabsch test, hit now once `0` (zero). The interface displayed by `aRMSD` in the terminal changes (figure 9), and you are able to trigger the refinement of the superposition with `-1` (minus one). The now following consecution of calling sub-routines is *recommended* to harvest the maximum of relevant data `aRMSD` provides.

  – Key-stroke `0` (zero) again opens the interactive Vtk-based visualizer (figure 10, left sub-figure). This adapted ball-stick representation displays *atom radii* of the atoms proportional to the *relative contribution* of said atoms to the global RMSD. The *atom colors* of the spheres scales to the absolute remaining difference of the two fit structures about said atom in Angstroms. The lateral scale offers an estimate of the latter.

    Some of the bonds depicted *might* bear a red band in the center. This is to indicate that the same bond in the reference model is significantly shorter, than in the tested model. Conversely, a green band indicates a bond that is longer. By default, the critical *length difference* to set these bands equals to 0.2 Angstrom.

    Clicking *on* a representation of one, two, three, or four atoms selects them to read-

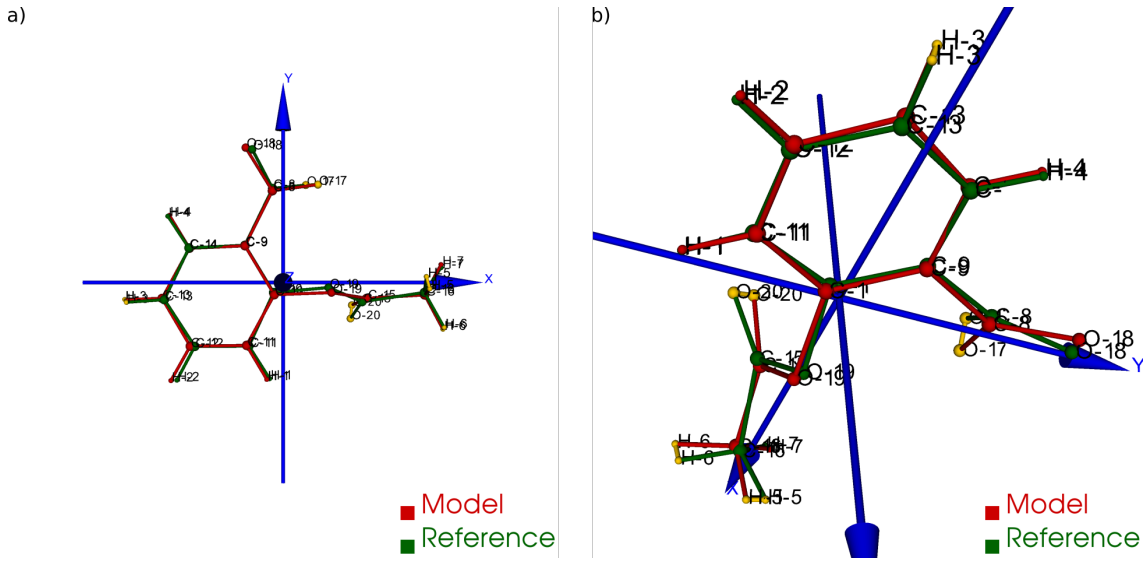

Figure 8: Successful application of the Hungarian algorithm on well aligned structures "model" and "reference". Yellow streaks mark atoms of different molecules remote from each other which subsequently will be considered by aRMSD as analogous to each other. a) Display in the default perspective of aRMSD. b) Altered perspective of the same "correlation".

out to the final RMSD data about the corresponding position; or corresponding difference in distance, angle; or dihedral angle between model and reference. These read-outs are non-permanent and provided *only* on the terminal (figure 11).

The underlying routine providing the readouts is agnostic about the atom type, allowing both the selection of hydrogens, as well as non-H atoms. The atoms of interest need not be adjacent, either, which may be of interest comparing distances and angles. Again, you close the visualizer with key-stroke `q`.

– A classical superposition display is obtained with key-stroke `1`. Model and reference are depicted by the visualizer (figure 10, right sub-figure) with the same color scheme as already known from the stage of prealignment. As in all other instances using the `vtk`-visualizer, the rendering may be saved as `*.png` (key-stroke `s`), and closed (with key-stroke `q`).

– With key-stroke `2`, an additional determination of statistics, and generation of synoptic diagrams is provided. This requires access to `matplotlib`, and opens a window separate from the therminal (figure 12).

  Currently, this analysis is organized in sub-plots that may partially overlap with each other if the new GUI starts. Increasing the dimension of the window renders the diagrams more legible – equally affecting the rendered permanent record.

  As usual for `matplotlib`, you have the options to zoom and pan within the sub-figures into particular regions of your interest. The complete analysis may be saved

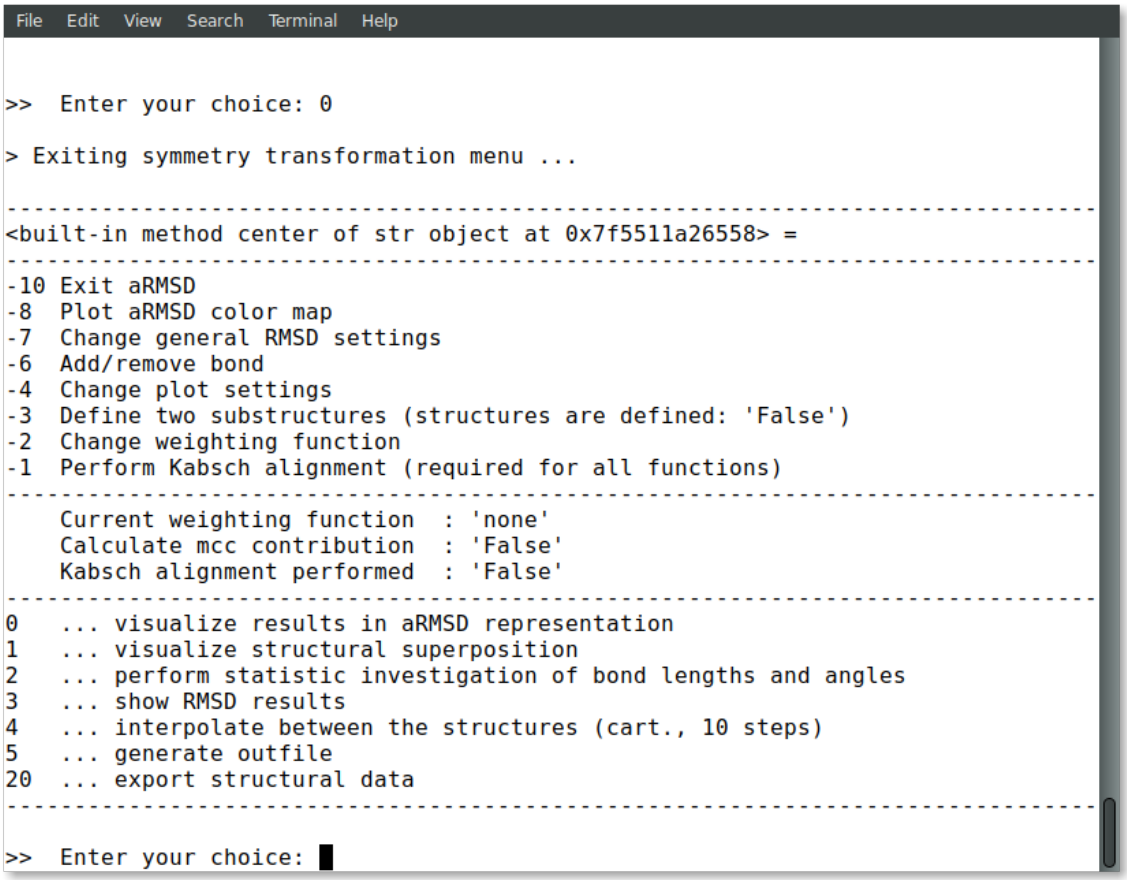

Figure 9: The CLI by aRMSD about the Kabsch test.

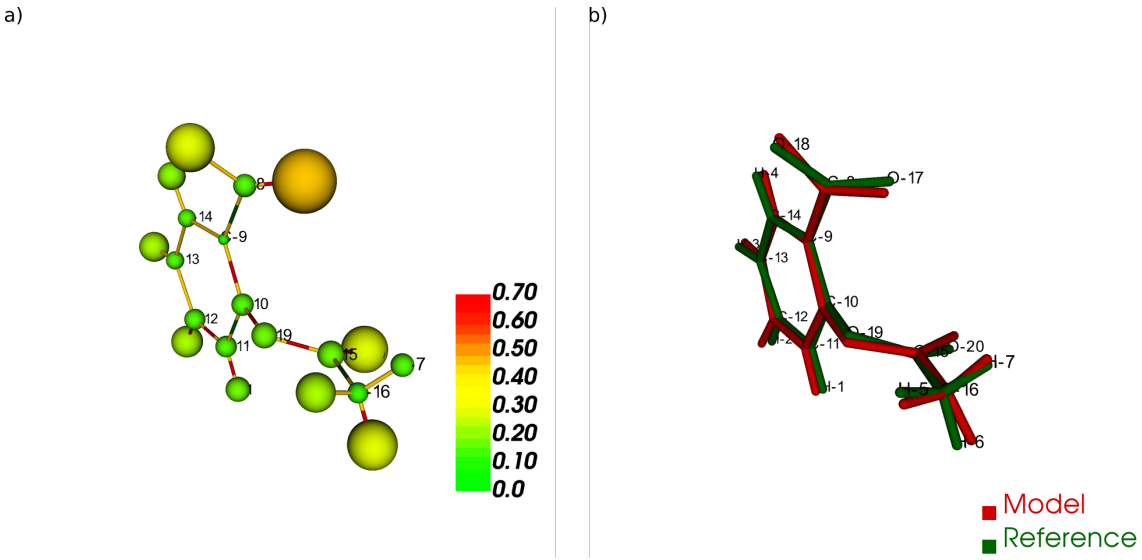

Figure 10: Structure display about the refined superposition of structure "model" (`M1.xyz`) and structure "reference" (`M2.xyz`) provided by `aRMSD`. a) Composite representation, where the *atom radii* scale to the relative, and the *atom colors* of the atom to the absolute contribution of said atoms to the global RMSD (reference scale in Angstroms). b) Wire-model superposition of the two models.

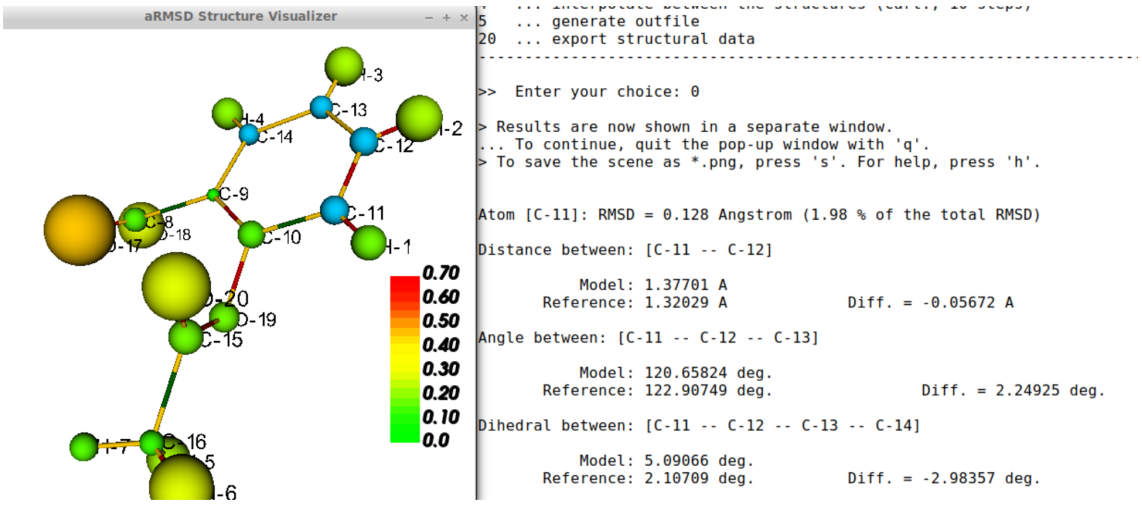

Figure 11: Example of subsequent selection of atom C11, C12, C13 and C14 to readout differences in position (or angle) in the refined superposition of the two structures `M1.xyz` and `M2.xyz`.

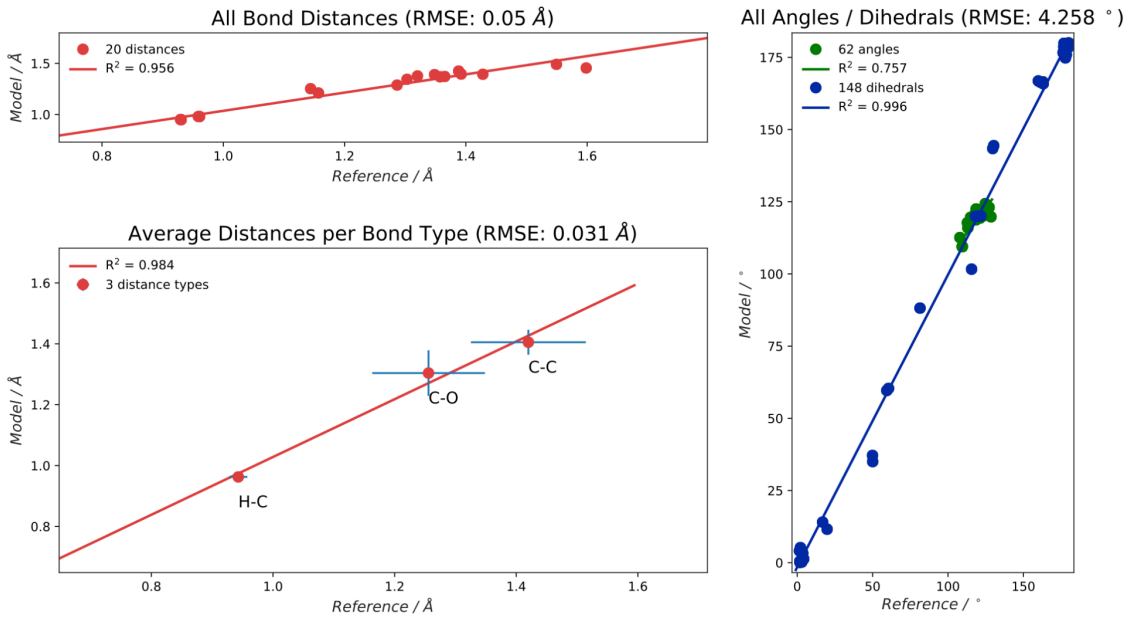

Figure 12: Synoptic statistics plots about the successfully comparison comparing the refined alignment of model `M1.xyz` and `M2.xyz` by `aRMSD`.

as bitmap (`*.jpeg`, `*.png` [default]), vector (`*.ps`, `*.eps`, `*.pdf`, `*.svg`), or tikz's `*.pgf`. By default, you have to define manually where `matplotlib` should deposit the drawings generated.

The window about the statistics plots may be closed either by mouse, or again key-stroke `q`.

– With call `3`, the program offers you a first decomposition about RMSD's contributions onto the terminal (figure 13). Even if you do not see these results when accessing `aRMSD` from a small terminal (80 × 24 chars), it is useful to invoke this sub-routine once – even blindly –, since *its results* will enter the permanent record log written.

– Key-stroke `5` initiates `aRMSD` to write a permanent record `aRMSD_log-file.out`. With exception of the structure representations and diagrams, this ASCII-file includes additional results of the similarity measurement, such as the rotation matrix applied to match the two structure models, or further figures of merit (e.g., cosine similarity, GARD similarity).

It equally provides you an insight about the quality of superposition *prior* and *after* the refinement. In the present case about a successful comparison of model `M1.xyz` with model `M2.xyz`, this is stated in line 48 onward about the initial best match retained:

```
* Details of the matching process:
    Structures were matched...                                    True
```

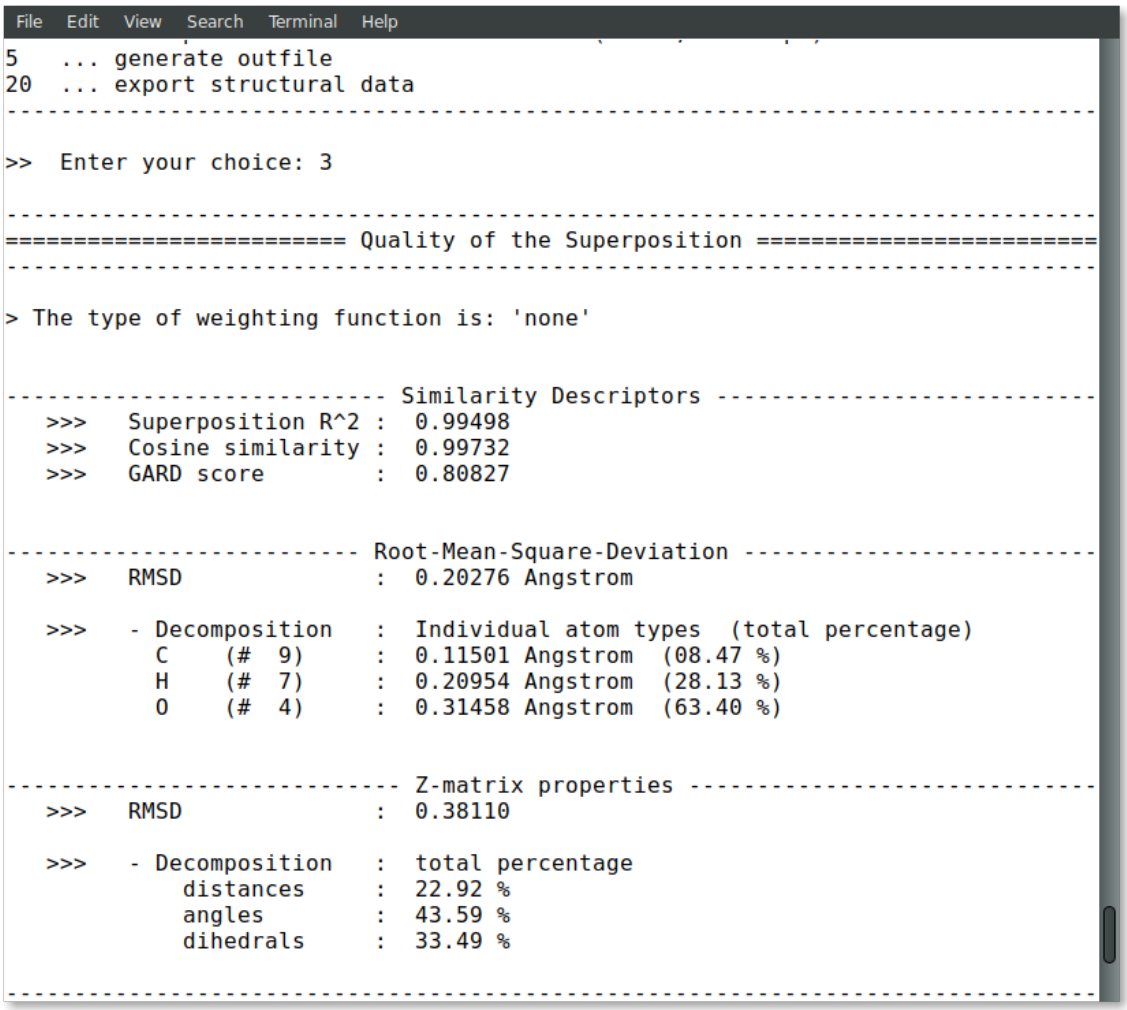

Figure 13: Terminal output of the refined superposition by aRMSD

```
Applied matching algorithm...                                  distance
Solver used for matching...                                   hungarian
Solution of the matching problem...                             regular
Number of highest deviations to be shown...                           5

The highest deviations were between the pairs...            [Angstrom]
                              H-3 -- H-3                         0.51023
                              H-5 -- H-5                         0.53943
                              H-6 -- H-6                         0.57067
                             O-20 -- O-20                        0.59816
                             O-17 -- O-17                        0.72202
The RMSD after the initial matching was [Angstrom]..             0.21397
```

and provides details about the sitution about the *then refined* superposition of the two model structures:

```
* Final Quality of the Superposition:

RMSD (Kabsch test, refined superposition [Angstrom])...          0.20276
Superposition R^2 (dimensionless)...                             0.99498
Cosine similarity (dimensionless)...                             0.99732
d values for the GARD calculation...                            0.3, 1.2
GARD score (dimensionless)...                                    0.80827

For an introduction into the GARD calculation, see J. C. Baber,
D. C. Thompson, J. B. Cross and C. Humblet, J. Chem. Inf. Model.,
2009, 49, 1889-1900, doi: 10.1021/ci9001074.
```

Last, but not least, a few words of caution:

- It is normal that performing the same computation a twice, with the same files, in a different operating system yields results *slighlty different* from each other, e.g. between Xubuntu (point release 18.04.1) and Debian 10 (testing / Buster).
- There are multiple "dialects" about the `*.pdb` format, which may require the model data you have to be converted into `*.xyz`, for example with `babel`[4] using a pattern of

  ```
  babel -ipdb input.pdb -oxyz converted.xyz
  ```

  As an example, the test data `M1.pdb` and `M2.pdb` were read successfully only to the Debian installation, but not to the Xubuntu analogue (cf. logs in the appendix).
- While retaining all other parameters equal, symmetry operations needed to perform the model alignment successfully about model data in `*.pdb` format may be different from the alignment about model data in `*.xyz`.

[4] Open Babel, `http://openbabel.org/wiki/Main_Page`. For further details, see by O'Boyle, N. M.; Banck, M.; James, C. A.; Morley, C.; Vandermeersch, T.; Hutchison, G. R. Open Babel: An open chemical toolbox. *J. Cheminf.* 2011, 3:33 (doi: 10.1186/1758-2946-3-33).

4 Example comparing two models unsuccessfully

The purpose of this section is to show *by strong contrast* to the previous chapter how to recognize an unsuccessfully performed analysis. Assuming you understood the general work-flow outlined in the section above, only a selected key points will be shown here. Again, the test data in question are `M1.xyz` and `M2.xyz`.

Starting from scratch, the model data are read again. To match the precedent case, all hydrogen atoms are retained for the analysis. Referring to figure 7, however, now *only* the symmetry operation of inversion is applied (hence, *intentionally omitting* the second operation of reflection in respect to the *xz*-plane).

The implementation of the Hungarian algorithm still relates the corresponding atoms successfully. However, both the increased number of yellow streaks as well their orientation *across* the structure models is a first warning sign (figure 14).

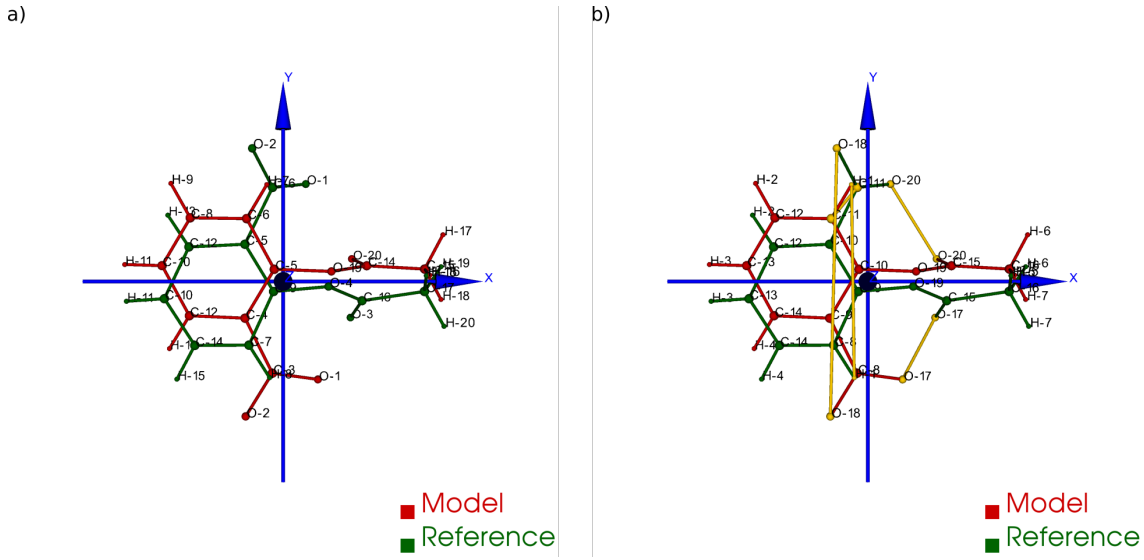

Figure 14: Example of an ill-fated comparison of structure `M1.xyz` with structure `M2.xyz` with `aRMSD`, step 1/3. a) The symmetry operation applied accounts only for inversion of the relative orientation of the two models. Consequently b), the number of atoms deemed analogous to each other yet marked by yellow streaks is higher, than in the "best match" (previous chapter). In addition, the streaks now pass largely *across* the structure models.

The subsequently performed refinement of the superposition consequently yields chemically unreasonable differences and pattern (figure 15), equally manifested in the statistics plots (figure 16).

To commplement the findings, the corresponding section in the log about the initial match states:

```
* Details of the matching process:
    Structures were matched...                                  True
```

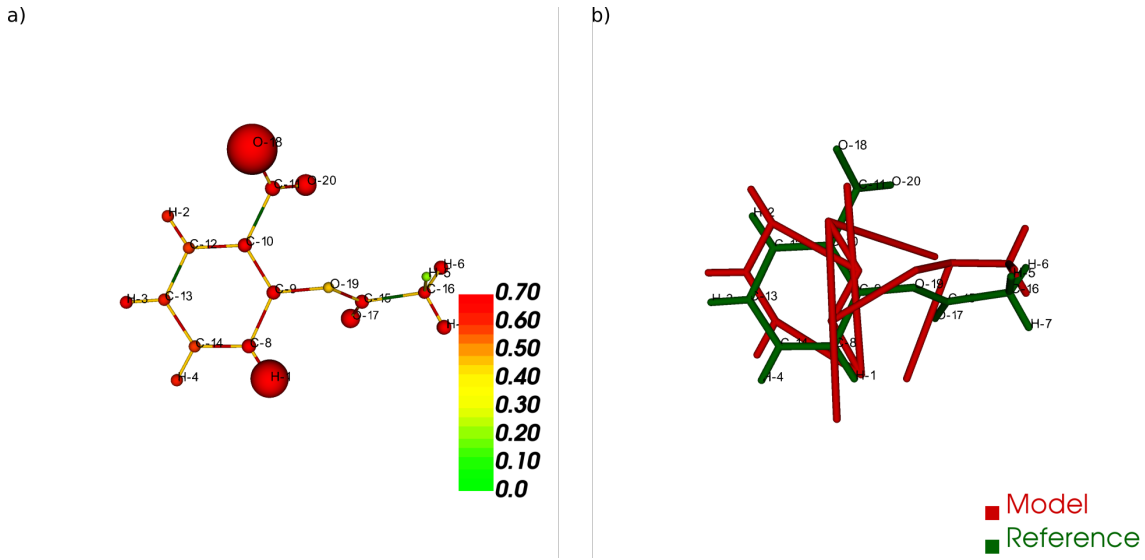

Figure 15: Example of an ill-fated comparison of structure `M1.xyz` with structure `M2.xyz` with aRMSD, step 2/3. a) Composite display, b) classical superposition representation.

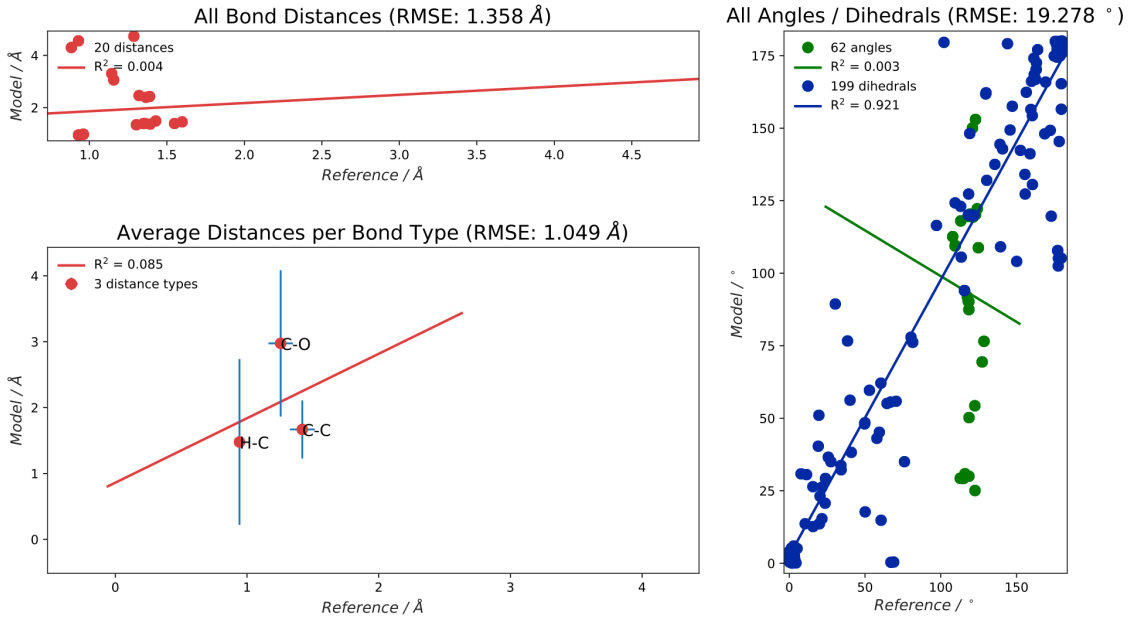

Figure 16: Example of an ill-fated comparison of structure `M1.xyz` with structure `M2.xyz` with aRMSD, 3/3. Synoptic statistics plots.

```
    Applied matching algorithm...                                    distance
    Solver used for matching...                                      hungarian
    Solution of the matching problem...                              regular
    Number of highest deviations to be shown...                      5

    The highest deviations were between the pairs...           [Angstrom]
                               C-11 -- C-11                     1.02336
                               O-17 -- O-17                     1.41194
                               O-20 -- O-20                     1.52207
                                H-1 -- H-1                      2.15521
                               O-18 -- O-18                     2.51862
    The RMSD after the initial matching was [Angstrom]..           2.01663
```

and provides details about the sitution about the *then refined* superposition of the two model structures:

```
* Final Quality of the Superposition:

    RMSD (Kabsch test, refined superposition [Angstrom])...          2.01343
    Superposition R^2 (dimensionless)...                             0.50549
    Cosine similarity (dimensionless)...                             0.77410
    d values for the GARD calculation...                             0.3, 1.2
    GARD score (dimensionless)...                                    0.47194

    For an introduction into the GARD calculation, see J. C. Baber,
    D. C. Thompson, J. B. Cross and C. Humblet, J. Chem. Inf. Model.,
    2009, 49, 1889-1900, doi: 10.1021/ci9001074.
```

5 Supplementary data

5.1 log-file by aRMSD about the successful comparison, xyz-data

The following is the *complete* log written by `aRMSD` about the successful comparison of model `M1.xyz` with model `M2.xyz`. Hosting system was Xubuntu 18.04 LTS (64 bit, point release 18.04.1).

```
+------------------------------------------------------------------------------+
|              aRMSD - automatic RMSD Calculator (version 0.9.8)               |
|                      Arne Wagner, Norwid Behrnd (2018)                       |
|                                                                              |
|    A brief description of the program can be found in the manual and in:     |
|            A. Wagner, PhD thesis, University of Heidelberg, 2015.            |
|                                                                              |
|    Cite this program by:                                                     |
|    A. Wagner, H.-J. Himmel, J. Chem. Inf. Model, 2017, 57, 428-438           |
```

```
|    (doi: 10.1021/acs.jcim.6b00516),                                          |
|    source (http://www.github.com/nbehrnd/armsd), and version used.           |
+------------------------------------------------------------------------------+

                                                                    03-Dec-2018


*** Log file about the superposition of structures ***

    "Model"...                                                          M1.xyz
    "Reference"...                                                      M2.xyz

* Consistency establishment between the structures:

  The basic approach is to subsequently remove hydrogen atoms
  until the same number of atoms is found in both molecules.
  If the number of atoms is identical and the atom types belong
  to the same group in the periodic table, the molecules are
  considered as consistent.

    No disorder in the structures was found.

    Initial number of atoms in "Model"...                    20  (7 H atoms)
    Initial number of atoms in "Reference"...                20  (7 H atoms)

    Consistency between the structures was established:
    The number of atoms in "Model"...                        20  (7 H atoms)
    The number of atoms in "Reference"...                    20  (7 H atoms)

    No further modifications were performed.

    Final global atom count (number of hydrogens retained)...        20  (7 H atoms)

* Transformation of the molecules into "Standard Orientation":
  1. The center of mass was shifted to the Cartesian origin.
  2. The moment of inertia tensor was constructed, diagonalized
     and the eigenvectors rotated on the x, y and z axes.

* Details of the matching process:
    Structures were matched...                                          True
    Applied matching algorithm...                                       distance
    Solver used for matching...                                         hungarian
    Solution of the matching problem...                                 regular
```

```
    Number of highest deviations to be shown...                    5

    The highest deviations were between the pairs...           [Angstrom]
                               H-3 -- H-3                        0.51023
                               H-5 -- H-5                        0.53943
                               H-6 -- H-6                        0.57067
                              O-20 -- O-20                       0.59816
                              O-17 -- O-17                       0.72202
    The RMSD after the initial matching was [Angstrom]..          0.21397

* Kabsch alignment:
    # General settings
    Substructures were defined...                                 False
    Weighting function for Kabsch algorithm...                    none
    Consideration of multi-center-contributions...                False

    # Differentiation criteria and color information
    Number of colors for aRMSD plot...                            19
    Maximum RMSD value for color projection [Angstrom]..          0.7
    Threshold for bond comparison [Angstrom]...                   0.02
    Number of distance pairs above threshold...                   12
    Percentage of the colored intersections...                    10.0
    Color for shorter bonds in "Model" vs. "Reference"...         #006400  [HEX]
    Color for longer bonds in "Model" vs. "Reference"...          #CD0000  [HEX]
    Number of bonds below threshold...                            12
    Color of "Model"...                                           #CD0000  [HEX]
    Color of "Reference"...                                       #006400  [HEX]

    Final rotation matrix from 'Standard Orientation':

           |-0.99991965  -0.01140142  +0.00554066|
     U  =  |-0.01160250  +0.99922073  -0.03772691|
           |-0.00510620  -0.03778816  -0.99927273|

    # This matrix aligns Model with Reference.
    # U already includes all custom symmetry operations!



* Final Quality of the Superposition:

    RMSD (Kabsch test, refined superposition [Angstrom])...       0.20276
    Superposition R^2 (dimensionless)...                          0.99498
```

```
    Cosine similarity (dimensionless)...                          0.99732
    d values for the GARD calculation...                          0.3, 1.2
    GARD score (dimensionless)...                                 0.80827

    For an introduction into the GARD calculation, see J. C. Baber,
    D. C. Thompson, J. B. Cross and C. Humblet, J. Chem. Inf. Model.,
    2009, 49, 1889-1900, doi: 10.1021/ci9001074.


* Decomposition into different atom types          absolute     relative
                                                  [Angstrom]      [%]
                                C    (#  9)         0.11501      (08.47)
                                H    (#  7)         0.20954      (28.13)
                                O    (#  4)         0.31458      (63.40)

    z-matrix properties:
    # z-matrices are created for both molecules, based on
    # (3 N - 1) bond distances, (3 N - 2) bond angles and
    # (3 N - 3) dihedral angles.  Both the total RMSD and
    # the relative contributions are calculated.
    RMSD [Angstrom]...                                            0.38110
    Contribution of distances...                                  22.92  [%]
    Contribution of angles...                                     43.59  [%]
    Contribution of dihedral angles...                            33.49  [%]

* Evaluation of structural parameters:
    # 1. The RMSE values are the root-mean-square errors
    #    between the corresponding properties of the two tructures.
    # 2. The R**2 values are the the correlation coefficients
    #    between the two data sets.

    Number of bonds...                                            20
    R**2 of linear correlation (dimensionless)...                 0.95580
    RMSE [Angstrom]...                                            0.05040

    Number of bond types...                                       3
    R**2 of linear correlation (dimensionless)...                 0.95580
    RMSE [Angstrom]...                                            0.03120

    Number of angles...                                           62
    R**2 of linear correlation (dimensionless)...                 0.75713
    RMSE [degrees]...                                             2.83420
```

```
    Number of dihedrals...                                          148
    R**2 of linear correlation (dimensionless)...                   0.99617
    RMSE [degrees]...                                               4.25830


*** End of log file ***
```

5.2 log-file by aRMSD about the unsuccessful comparison, xyz-data

The following is the *complete* log written by aRMSD about the unsuccessful comparison of model M1.xyz with model M2.xyz. Hosting system was Xubuntu 18.04 LTS (64 bit, point release 18.04.1).

```
+-------------------------------------------------------------------------------+
|              aRMSD - automatic RMSD Calculator (version 0.9.8)                |
|                      Arne Wagner, Norwid Behrnd (2018)                        |
|                                                                               |
|    A brief description of the program can be found in the manual and in:      |
|            A. Wagner, PhD thesis, University of Heidelberg, 2015.             |
|                                                                               |
|    Cite this program by:                                                      |
|    A. Wagner, H.-J. Himmel, J. Chem. Inf. Model, 2017, 57, 428-438            |
|    (doi: 10.1021/acs.jcim.6b00516),                                           |
|    source (http://www.github.com/nbehrnd/armsd), and version used.            |
+-------------------------------------------------------------------------------+

                                                                    03-Dec-2018


*** Log file about the superposition of structures ***

    "Model"...                                                          M1.xyz
    "Reference"...                                                      M2.xyz

* Consistency establishment between the structures:

  The basic approach is to subsequently remove hydrogen atoms
  until the same number of atoms is found in both molecules.
  If the number of atoms is identical and the atom types belong
  to the same group in the periodic table, the molecules are
  considered as consistent.

    No disorder in the structures was found.

    Initial number of atoms in "Model"...                       20  (7 H atoms)
    Initial number of atoms in "Reference"...                   20  (7 H atoms)

    Consistency between the structures was established:
    The number of atoms in "Model"...                           20  (7 H atoms)
    The number of atoms in "Reference"...                       20  (7 H atoms)

    No further modifications were performed.
```

```
    Final global atom count (number of hydrogens retained)...        20  (7 H atoms)

* Transformation of the molecules into "Standard Orientation":
  1. The center of mass was shifted to the Cartesian origin.
  2. The moment of inertia tensor was constructed, diagonalized
     and the eigenvectors rotated on the x, y and z axes.

* Details of the matching process:
    Structures were matched...                                    True
    Applied matching algorithm...                                 distance
    Solver used for matching...                                   hungarian
    Solution of the matching problem...                           regular
    Number of highest deviations to be shown...                   5

    The highest deviations were between the pairs...           [Angstrom]
                              C-11 -- C-11                      1.02336
                              O-17 -- O-17                      1.41194
                              O-20 -- O-20                      1.52207
                               H-1 -- H-1                       2.15521
                              O-18 -- O-18                      2.51862
    The RMSD after the initial matching was [Angstrom]..           2.01663

* Kabsch alignment:
    # General settings
    Substructures were defined...                                 False
    Weighting function for Kabsch algorithm...                    none
    Consideration of multi-center-contributions...                False

    # Differentiation criteria and color information
    Number of colors for aRMSD plot...                            19
    Maximum RMSD value for color projection [Angstrom]..          0.7
    Threshold for bond comparison [Angstrom]...                   0.02
    Number of distance pairs above threshold...                   16
    Percentage of the colored intersections...                    10.0
    Color for shorter bonds in "Model" vs. "Reference"...         #006400  [HEX]
    Color for longer bonds in "Model" vs. "Reference"...          #CD0000  [HEX]
    Number of bonds below threshold...                            16
    Color of "Model"...                                           #CD0000  [HEX]
    Color of "Reference"...                                       #006400  [HEX]

    Final rotation matrix from 'Standard Orientation':
```

```
        |-0.99890300  -0.04569042  +0.01025632|
 U  =   |+0.04565583  -0.99895081  -0.00358193|
        |-0.01040922  +0.00310974  -0.99994099|

    # This matrix aligns Model with Reference.
    # U already includes all custom symmetry operations!
```

```
* Final Quality of the Superposition:

    RMSD (Kabsch test, refined superposition [Angstrom])...          2.01343
    Superposition R^2 (dimensionless)...                             0.50549
    Cosine similarity (dimensionless)...                             0.77410
    d values for the GARD calculation...                             0.3, 1.2
    GARD score (dimensionless)...                                    0.47194

    For an introduction into the GARD calculation, see J. C. Baber,
    D. C. Thompson, J. B. Cross and C. Humblet, J. Chem. Inf. Model.,
    2009, 49, 1889-1900, doi: 10.1021/ci9001074.
```

```
* Decomposition into different atom types          absolute     relative
                                                  [Angstrom]      [%]
                              C    (#  9)          0.86236      (04.46)
                              H    (#  7)          1.88536      (21.32)
                              O    (#  4)          3.51793      (74.22)

    z-matrix properties:
    # z-matrices are created for both molecules, based on
    # (3 N - 1) bond distances, (3 N - 2) bond angles and
    # (3 N - 3) dihedral angles.  Both the total RMSD and
    # the relative contributions are calculated.
    RMSD [Angstrom]...                                               0.51559
    Contribution of distances...                                     27.97  [%]
    Contribution of angles...                                        56.78  [%]
    Contribution of dihedral angles...                               15.24  [%]

* Evaluation of structural parameters:
    # 1. The RMSE values are the root-mean-square errors
    #    between the corresponding properties of the two tructures.
    # 2. The R**2 values are the the correlation coefficients
    #    between the two data sets.
```

```
    Number of bonds...                                      20
    R**2 of linear correlation (dimensionless)...           0.00370
    RMSE [Angstrom]...                                      1.35760

    Number of bond types...                                 3
    R**2 of linear correlation (dimensionless)...           0.00370
    RMSE [Angstrom]...                                      1.04920

    Number of angles...                                     62
    R**2 of linear correlation (dimensionless)...           0.00251
    RMSE [degrees]...                                       43.83380

    Number of dihedrals...                                  199
    R**2 of linear correlation (dimensionless)...           0.92064
    RMSE [degrees]...                                       19.27750


*** End of log file ***
```

5.3 log-file by aRMSD about the successful comparison, pdb-data

In contrast to the `*.xyz` format, there are multiple "dialects" about the `*.pdb` format, which may represent an obstacle already loading the model data. At the moment, the cause is not yet understood. A low-level resort may be to convert the files into the `*.xyz` format, e.g. with `babel` in a pattern of

```
babel -ipdb input.pdb -oxyz output.xyz
```

In present case, loading the `*.pdb` successfully was possible in the reference system (Debian 10), but not with Xubuntu 18.04 (point release 18.04.1), despite the installations of `openbabel` in both systems seemingly were identical.

The following is the *complete* log written by `aRMSD` about the successful comparison of model `M1.pdb` with model `M2.pdb`.

```
+-------------------------------------------------------------------------------+
|              aRMSD - automatic RMSD Calculator (version 0.9.8)                |
|                      Arne Wagner, Norwid Behrnd (2018)                        |
|                                                                               |
|    A brief description of the program can be found in the manual and in:      |
|            A. Wagner, PhD thesis, University of Heidelberg, 2015.             |
|                                                                               |
|    Cite this program by:                                                      |
|    A. Wagner, H.-J. Himmel, J. Chem. Inf. Model, 2017, 57, 428-438            |
|    (doi: 10.1021/acs.jcim.6b00516),                                           |
|    source (http://www.github.com/nbehrnd/armsd), and version used.            |
+-------------------------------------------------------------------------------+

                                                                    03-Dec-2018


*** Log file about the superposition of structures ***

    "Model"...                                                          M1.xyz
    "Reference"...                                                      M2.xyz

* Consistency establishment between the structures:

  The basic approach is to subsequently remove hydrogen atoms
  until the same number of atoms is found in both molecules.
  If the number of atoms is identical and the atom types belong
  to the same group in the periodic table, the molecules are
  considered as consistent.

    No disorder in the structures was found.
```

```
    Initial number of atoms in "Model"...                    20  (7 H atoms)
    Initial number of atoms in "Reference"...                20  (7 H atoms)

    Consistency between the structures was established:
    The number of atoms in "Model"...                        20  (7 H atoms)
    The number of atoms in "Reference"...                    20  (7 H atoms)

    No further modifications were performed.

    Final global atom count (number of hydrogens retained)...     20  (7 H atoms)

* Transformation of the molecules into "Standard Orientation":
  1. The center of mass was shifted to the Cartesian origin.
  2. The moment of inertia tensor was constructed, diagonalized
     and the eigenvectors rotated on the x, y and z axes.

* Details of the matching process:
    Structures were matched...                               True
    Applied matching algorithm...                            distance
    Solver used for matching...                              hungarian
    Solution of the matching problem...                      regular
    Number of highest deviations to be shown...              5

    The highest deviations were between the pairs...        [Angstrom]
                               H-3 -- H-3                     0.51023
                               H-5 -- H-5                     0.53943
                               H-6 -- H-6                     0.57067
                              O-20 -- O-20                    0.59816
                              O-17 -- O-17                    0.72202
    The RMSD after the initial matching was [Angstrom]..        0.21397

* Kabsch alignment:
    # General settings
    Substructures were defined...                            False
    Weighting function for Kabsch algorithm...               none
    Consideration of multi-center-contributions...           False

    # Differentiation criteria and color information
    Number of colors for aRMSD plot...                       19
    Maximum RMSD value for color projection [Angstrom]..     0.7
    Threshold for bond comparison [Angstrom]...              0.02
    Number of distance pairs above threshold...              12
```

```
    Percentage of the colored intersections...                    10.0
    Color for shorter bonds in "Model" vs. "Reference"...         #006400  [HEX]
    Color for longer bonds in "Model" vs. "Reference"...          #CD0000  [HEX]
    Number of bonds below threshold...                            12
    Color of "Model"...                                           #CD0000  [HEX]
    Color of "Reference"...                                       #006400  [HEX]

    Final rotation matrix from 'Standard Orientation':

           |-0.99991965  -0.01140142  +0.00554066|
     U  =  |-0.01160250  +0.99922073  -0.03772691|
           |-0.00510620  -0.03778816  -0.99927273|

    # This matrix aligns Model with Reference.
    # U already includes all custom symmetry operations!



* Final Quality of the Superposition:

    RMSD (Kabsch test, refined superposition [Angstrom])...       0.20276
    Superposition R^2 (dimensionless)...                          0.99498
    Cosine similarity (dimensionless)...                          0.99732
    d values for the GARD calculation...                          0.3, 1.2
    GARD score (dimensionless)...                                 0.80827

    For an introduction into the GARD calculation, see J. C. Baber,
    D. C. Thompson, J. B. Cross and C. Humblet, J. Chem. Inf. Model.,
    2009, 49, 1889-1900, doi: 10.1021/ci9001074.


* Decomposition into different atom types          absolute     relative
                                                  [Angstrom]     [%]
                                C    (#  9)         0.11501     (08.47)
                                H    (#  7)         0.20954     (28.13)
                                O    (#  4)         0.31458     (63.40)

    z-matrix properties:
    # z-matrices are created for both molecules, based on
    # (3 N - 1) bond distances, (3 N - 2) bond angles and
    # (3 N - 3) dihedral angles.  Both the total RMSD and
    # the relative contributions are calculated.
    RMSD [Angstrom]...                                            0.38110
```

```
    Contribution of distances...                              22.92  [%]
    Contribution of angles...                                 43.59  [%]
    Contribution of dihedral angles...                        33.49  [%]

* Evaluation of structural parameters:
    # 1. The RMSE values are the root-mean-square errors
    #    between the corresponding properties of the two tructures.
    # 2. The R**2 values are the the correlation coefficients
    #    between the two data sets.

    Number of bonds...                                        20
    R**2 of linear correlation (dimensionless)...             0.95580
    RMSE [Angstrom]...                                        0.05040

    Number of bond types...                                   3
    R**2 of linear correlation (dimensionless)...             0.95580
    RMSE [Angstrom]...                                        0.03120

    Number of angles...                                       62
    R**2 of linear correlation (dimensionless)...             0.75713
    RMSE [degrees]...                                         2.83420

    Number of dihedrals...                                    148
    R**2 of linear correlation (dimensionless)...             0.99617
    RMSE [degrees]...                                         4.25830


*** End of log file ***
```

5.4 complete *terminal log* by aRMSD for the successful comparison of xyz-data

The following is the *complete* output `aRMSD` generates on the terminal while comparing model `M1.xyz` with model `M2.xyz` *successfully*. Operating system was Xubuntu 18.04.1.

```
================================================================================
                          aRMSD (version 0.9.8, 2018)
================================================================================
               A. Wagner, University of Heidelberg (2015, 2017),
                          forked by N. Behrnd (2018)

--------------------------------- Description ---------------------------------
Key features:
* Parses data from various file formats
* Establishes consistency and matches coordinate sequences of two molecules
* Aligns two molecular structures based on the Kabsch algorithm
* Supports different weighting functions for the superposition
* Supports error propagation for experimental structures
* Generates different visualization types of the superposition results
* Writes outfiles that can be passed to other programs
* The original version was created by A. Wagner under Windows.  You find it
      hosted on GitHub: https://github.com/armsd/aRMSD.
* You are using a derivative fork based on the former, developed under Linux
      by N. Behrnd, hosted on GitHub: https://github.com/nbehrnd/aRMSD.

*** Cite this program as:
    A. Wagner, H.-J. Himmel, J. Chem. Inf. Model, 2017, 57, 428-438
    (doi: 10.1021/acs.jcim.6b00516); with address and version of aRMSD used.

Release dates of the individual modules:
- core module:            '2018-10-24'
- plot module:            '2016-11-03'
- log  module:            '2018-11-28'

Module check:
- numpy                 '1.13.3'
- VTK                   '6.3.0'
- matplotlib            '2.1.1'
- uncertainties         '2.4.4'
- openbabel             '2.3.2'
--------------------------------------------------------------------------------

Enter the file name with extension for the first file (comp./model)
```

```
>> M1.xyz

> 'M1.xyz' has been loaded successfully! (#Atoms: 20)

Enter the file name with extension for the second file (exp./reference)
>> M2.xyz

> 'M2.xyz' has been loaded successfully! (#Atoms: 20)
--------------------------------------------------------------------------------
... Files have been loaded!

--------------------------------------------------------------------------------
> Checking for coordinate standard deviations...
... No standard deviations were found!
--------------------------------------------------------------------------------

  Checking length unit of xyz coordinates ...
  The coordinate unit is [Angstrom]

  Checking length unit of xyz coordinates ...
  The coordinate unit is [Angstrom]

> The current status was saved successfully!


--------------------------------------------------------------------------------
================ Consistency Checks and Structural Modification ================
--------------------------------------------------------------------------------

> Performing consistency checks ... (Number of atoms: 20, 20)
  There are (7 & 7) H atoms in the molecules

> The structures of both molecules are consistent.

--------------------------------------------------------------------------------
    What should happen to the remaining 7 H-atoms?
--------------------------------------------------------------------------------
    Info: The exclusion of H-atoms in RMSD calculations is recommended if
          they were not located and refined in the X-ray experiment
--------------------------------------------------------------------------------
0   ... remove all hydrogen atoms (7)
3   ... keep all hydrogen atoms
--------------------------------------------------------------------------------
```

```
>>  Enter your choice: 3

> The molecules were rotated into 'Standard Orientation' ...

> The current status was saved successfully!

-------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ==================
-------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
-------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'False'
-------------------------------------------------------------------------------
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
-------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
-------------------------------------------------------------------------------

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.

>>  Enter your choice: 1

> Inversion of 'Model' structure at the origin of the coordinate system ...
```

```
--------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ===================
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
--------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'False'
--------------------------------------------------------------------------------
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.

>>  Enter your choice: 3

> Reflection of 'Model' structure at the xz-plane ...

--------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ===================
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
```

```
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
--------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'False'
--------------------------------------------------------------------------------
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.

>>  Enter your choice: 10

> The current status was saved successfully!

--------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ===================
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
--------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'False'
--------------------------------------------------------------------------------
```

```
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

>>  Enter your choice: -1

--------------------------------------------------------------------------------

        The geometric RMSD of the current alignment is:  0.214 A

                The 5 most disordered atom pairs are:
               Entry                     Pair                  Distance / A
                 5                  H-3 -- H-3                0.510
                 4                  H-5 -- H-5                0.539
                 3                  H-6 -- H-6                0.571
                 2                 O-20 -- O-20               0.598
                 1                 O-17 -- O-17               0.722

--------------------------------------------------------------------------------
================== Symmetry Adjustments & Sequence Matching ==================
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
--------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'True'
--------------------------------------------------------------------------------
0   ... exit the menu (no return)
```

```
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.

>>  Enter your choice: 10

> The current status was saved successfully!

--------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ===================
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
--------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'True'
--------------------------------------------------------------------------------
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
```

```
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

>>  Enter your choice: 0

> Exiting symmetry transformation menu ...

--------------------------------------------------------------------------------
<built-in method center of str object at 0x7feaeab0aad8> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'False'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: -1

--------------------------------------------------------------------------------
======================== Quality of the Superposition ========================
--------------------------------------------------------------------------------

> The type of weighting function is: 'none'
```

```
---------------------------- Similarity Descriptors ----------------------------
   >>>   Superposition R^2 :  0.99498
   >>>   Cosine similarity :  0.99732
   >>>   GARD score        :  0.80827


-------------------------- Root-Mean-Square-Deviation --------------------------
   >>>   RMSD              :  0.20276 Angstrom

   >>>   - Decomposition   :  Individual atom types  (total percentage)
           C    (#  9)     :  0.11501 Angstrom  (08.47 %)
           H    (#  7)     :  0.20954 Angstrom  (28.13 %)
           O    (#  4)     :  0.31458 Angstrom  (63.40 %)


------------------------------ Z-matrix properties -----------------------------
   >>>   RMSD              :  0.38110

   >>>   - Decomposition   :  total percentage
              distances     :  22.92 %
              angles        :  43.59 %
              dihedrals     :  33.49 %

--------------------------------------------------------------------------------
<built-in method center of str object at 0x7feaeab0aad8> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
```

```
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: 0

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.

--------------------------------------------------------------------------------
<built-in method center of str object at 0x7feaeab0aad8> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: 1

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.
```

```
--------------------------------------------------------------------------------
<built-in method center of str object at 0x7feaeab0aad8> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: 2

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.


---------------- The Highest Deviations in Internal Coordinates ----------------
The 3 highest deviations are printed below
Entries are: Atoms, values in the Model and Reference, difference
--------------------------------------------------------------------------------
 >> Bonds (in Angstrom):
    1.  [C-15, C-16] 1.455 1.598        Diff. 0.143
    2.  [C-8, O-17] 1.252 1.144        Diff. -0.108
    3.  [C-8, C-9] 1.49 1.549        Diff. 0.059
--------------------------------------------------------------------------------
 >> Bond angles (in deg.):
    1.  [O-18, C-8, O-17] 119.78 128.521        Diff. 8.741
    2.  [O-17, C-8, O-18] 119.78 128.521        Diff. 8.741
```

```
    3.  [C-9, C-8, O-18] 117.731 112.838        Diff. -4.893
--------------------------------------------------------------------------------
 >> Dihedral angles (in deg.):
    1.  [C-14, C-9, C-8, O-18] 35.01 50.069        Diff. 15.059
    2.  [O-18, C-8, C-9, C-14] 35.01 50.069        Diff. 15.059
    3.  [O-17, C-8, C-9, C-14] 144.42 130.333        Diff. -14.087
--------------------------------------------------------------------------------

--------------------------------------------------------------------------------
<built-in method center of str object at 0x7feaeab0aad8> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: 3

--------------------------------------------------------------------------------
======================== Quality of the Superposition ========================
--------------------------------------------------------------------------------

> The type of weighting function is: 'none'


---------------------------- Similarity Descriptors ----------------------------
```

```
   >>>   Superposition R^2 :  0.99498
   >>>   Cosine similarity :  0.99732
   >>>   GARD score        :  0.80827


-------------------------- Root-Mean-Square-Deviation --------------------------
   >>>   RMSD              :  0.20276 Angstrom

   >>>   - Decomposition   :  Individual atom types  (total percentage)
           C    (#  9)     :  0.11501 Angstrom  (08.47 %)
           H    (#  7)     :  0.20954 Angstrom  (28.13 %)
           O    (#  4)     :  0.31458 Angstrom  (63.40 %)


------------------------------ Z-matrix properties -------------------------------
   >>>   RMSD              :  0.38110

   >>>   - Decomposition   :  total percentage
              distances     :  22.92 %
              angles        :  43.59 %
              dihedrals     :  33.49 %

--------------------------------------------------------------------------------
<built-in method center of str object at 0x7feaeab0aad8> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
```

```
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: 5

> A logfile (aRMSD_logfile.out) has been written successfully!

--------------------------------------------------------------------------------
<built-in method center of str object at 0x7feaeab0aad8> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: -10

--------------------------------------------------------------------------------
========================= Normal program termination ==========================
--------------------------------------------------------------------------------
```

5.5 complete *terminal log* by aRMSD for the successful comparison of pdb-data

The following is the *complete* output `aRMSD` generates on the terminal while comparing model `M1.pdb` with model `M2.pdb` *successfully*. Operating system was Debian 10 (testing / Buster).

```
================================================================================
                          aRMSD (version 0.9.8, 2018)
================================================================================
               A. Wagner, University of Heidelberg (2015, 2017),
                           forked by N. Behrnd (2018)

--------------------------------- Description ---------------------------------
Key features:
* Parses data from various file formats
* Establishes consistency and matches coordinate sequences of two molecules
* Aligns two molecular structures based on the Kabsch algorithm
* Supports different weighting functions for the superposition
* Supports error propagation for experimental structures
* Generates different visualization types of the superposition results
* Writes outfiles that can be passed to other programs
* The original version was created by A. Wagner under Windows.  You find it
      hosted on GitHub: https://github.com/armsd/aRMSD.
* You are using a derivative fork based on the former, developed under Linux
      by N. Behrnd, hosted on GitHub: https://github.com/nbehrnd/aRMSD.

*** Cite this program as:
    A. Wagner, H.-J. Himmel, J. Chem. Inf. Model, 2017, 57, 428-438
    (doi: 10.1021/acs.jcim.6b00516); with address and version of aRMSD used.

Release dates of the individual modules:
- core module:            '2018-10-24'
- plot module:            '2016-11-03'
- log  module:            '2018-11-28'

Module check:
- numpy                 '1.14.5'
- VTK                   '6.3.0'
- matplotlib            '2.2.2'
- uncertainties         '3.0.2'
- openbabel             '2.4.1'
--------------------------------------------------------------------------------

Enter the file name with extension for the first file (comp./model)
```

```
>> M1.cif

> ERROR: File type is not supported by openbabel!

Enter the file name with extension for the first file (comp./model)
>> M1.pdb

> 'M1.pdb' has been loaded successfully! (#Atoms: 20)

Enter the file name with extension for the second file (exp./reference)
>> M2.pdb

> 'M2.pdb' has been loaded successfully! (#Atoms: 20)
--------------------------------------------------------------------------------
... Files have been loaded!

--------------------------------------------------------------------------------
> Checking for coordinate standard deviations...
... No standard deviations were found!
--------------------------------------------------------------------------------

  Checking length unit of xyz coordinates ...
  The coordinate unit is [Angstrom]

  Checking length unit of xyz coordinates ...
  The coordinate unit is [Angstrom]

> The current status was saved successfully!


--------------------------------------------------------------------------------
================ Consistency Checks and Structural Modification ================
--------------------------------------------------------------------------------

> Performing consistency checks ... (Number of atoms: 20, 20)
  There are (7 & 7) H atoms in the molecules

> The structures of both molecules are consistent.

--------------------------------------------------------------------------------
    What should happen to the remaining 7 H-atoms?
--------------------------------------------------------------------------------
    Info: The exclusion of H-atoms in RMSD calculations is recommended if
```

```
          they were not located and refined in the X-ray experiment
--------------------------------------------------------------------------------
0   ... remove all hydrogen atoms (7)
3   ... keep all hydrogen atoms
--------------------------------------------------------------------------------

>>  Enter your choice: 3

> The molecules were rotated into 'Standard Orientation' ...

> The current status was saved successfully!

--------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ===================
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
--------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'False'
--------------------------------------------------------------------------------
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.
```

```
>>  Enter your choice: 1

> Inversion of 'Model' structure at the origin of the coordinate system ...

--------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ===================
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
--------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'False'
--------------------------------------------------------------------------------
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.

>>  Enter your choice: 2

> Reflection of 'Model' structure at the xy-plane ...

--------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ===================
```

```
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
--------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'False'
--------------------------------------------------------------------------------
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.

>>  Enter your choice: 10

> The current status was saved successfully!

--------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ===================
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
```

```
--------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'False'
--------------------------------------------------------------------------------
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

>>  Enter your choice: -1

--------------------------------------------------------------------------------

        The geometric RMSD of the current alignment is:  0.214 A

                The 5 most disordered atom pairs are:
               Entry                      Pair                  Distance / A
                 5                    H-3 -- H-3                0.511
                 4                    H-5 -- H-5                0.539
                 3                    H-6 -- H-6                0.571
                 2                   O-20 -- O-20               0.598
                 1                   O-17 -- O-17               0.722

--------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ===================
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
--------------------------------------------------------------------------------
```

```
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'True'
--------------------------------------------------------------------------------
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.

>>  Enter your choice: 10

> The current status was saved successfully!

--------------------------------------------------------------------------------
=================== Symmetry Adjustments & Sequence Matching ===================
--------------------------------------------------------------------------------
-6  Set number of deviations which are highlighted in the plot (current = 5)
-5  Load the saved status (save point available: 'True')
-4  Change plot settings
-3  Manually swap atoms in Model structure
-2  Change matching algorithm or solver
-1  Match molecular sequences based on current alignment
--------------------------------------------------------------------------------
    Current matching algorithm  : 'distance'
    Current matching solver     : 'hungarian'
    Structures were matched     : 'True'
--------------------------------------------------------------------------------
0   ... exit the menu (no return)
1   ... inversion at the origin
2   ... reflection at the xy plane
```

```
3   ... reflection at the xz plane
4   ... reflection at the yz plane
5   ... rotation around the x axis
6   ... rotation around the y axis
7   ... rotation around the z axis
8   ... show the molecules again
--------------------------------------------------------------------------------
10  ... save current changes (status was saved: 'True')
20  ... export structures
--------------------------------------------------------------------------------

>>  Enter your choice: 0

> Exiting symmetry transformation menu ...

--------------------------------------------------------------------------------
<built-in method center of str object at 0x7f7ba4445240> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'False'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: -1

--------------------------------------------------------------------------------
```

```
======================== Quality of the Superposition ========================
------------------------------------------------------------------------------

> The type of weighting function is: 'none'


---------------------------- Similarity Descriptors ----------------------------
   >>>   Superposition R^2 :  0.99498
   >>>   Cosine similarity :  0.99731
   >>>   GARD score        :  0.80826


-------------------------- Root-Mean-Square-Deviation --------------------------
   >>>   RMSD              :  0.20276 Angstrom

   >>>   - Decomposition   :  Individual atom types  (total percentage)
           C    (#  9)     :  0.11507 Angstrom  (08.48 %)
           H    (#  7)     :  0.20956 Angstrom  (28.14 %)
           O    (#  4)     :  0.31451 Angstrom  (63.38 %)


------------------------------ Z-matrix properties -----------------------------
   >>>   RMSD              :  0.38077

   >>>   - Decomposition   :  total percentage
              distances     :  22.96 %
              angles        :  43.37 %
              dihedrals     :  33.67 %

------------------------------------------------------------------------------
<built-in method center of str object at 0x7f7ba4445240> =
------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
```

```
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: 0

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.

--------------------------------------------------------------------------------
<built-in method center of str object at 0x7f7ba4445240> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: 1
```

```
> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.
> To save the scene as *.png, press 's'.

--------------------------------------------------------------------------------
<built-in method center of str object at 0x7f7ba4445240> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: 2

> Results are now shown in a separate window.
... To continue, quit the pop-up window with 'q'.


---------------- The Highest Deviations in Internal Coordinates ----------------
The 3 highest deviations are printed below
Entries are: Atoms, values in the Model and Reference, difference
--------------------------------------------------------------------------------
 >> Bonds (in Angstrom):
    1.  [C-15, C-16] 1.454 1.598        Diff. 0.14400000000000013
    2.  [C-8, O-17] 1.253 1.143        Diff. -0.10999999999999988
```

```
    3.  [C-8, C-9] 1.491 1.55        Diff. 0.05899999999999994
--------------------------------------------------------------------------------
 >> Bond angles (in deg.):
    1.  [O-18, C-8, O-17] 119.817 128.56        Diff. 8.74300000000001
    2.  [O-17, C-8, O-18] 119.817 128.56        Diff. 8.74300000000001
    3.  [C-9, C-8, O-18] 117.728 112.809        Diff. -4.918999999999997
--------------------------------------------------------------------------------
 >> Dihedral angles (in deg.):
    1.  [C-14, C-9, C-8, O-18] 35.066 50.081        Diff. 15.015
    2.  [O-18, C-8, C-9, C-14] 35.066 50.081        Diff. 15.015
    3.  [C-14, C-9, C-8, O-17] 144.442 130.267        Diff. -14.175000000000011
--------------------------------------------------------------------------------


--------------------------------------------------------------------------------
<built-in method center of str object at 0x7f7ba4445240> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
--------------------------------------------------------------------------------

>>  Enter your choice: 3

--------------------------------------------------------------------------------
======================== Quality of the Superposition ========================
--------------------------------------------------------------------------------
```

```
> The type of weighting function is: 'none'


---------------------------- Similarity Descriptors ----------------------------
   >>>   Superposition R^2 :  0.99498
   >>>   Cosine similarity :  0.99731
   >>>   GARD score        :  0.80826


-------------------------- Root-Mean-Square-Deviation --------------------------
   >>>   RMSD              :  0.20276 Angstrom

   >>>   - Decomposition   :  Individual atom types  (total percentage)
           C    (#  9)     :  0.11507 Angstrom  (08.48 %)
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           O    (#  4)     :  0.31451 Angstrom  (63.38 %)


------------------------------ Z-matrix properties -----------------------------
   >>>   RMSD              :  0.38077

   >>>   - Decomposition   :  total percentage
             distances     :  22.96 %
             angles        :  43.37 %
             dihedrals     :  33.67 %

--------------------------------------------------------------------------------
<built-in method center of str object at 0x7f7ba4445240> =
--------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
--------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
--------------------------------------------------------------------------------
```

```
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
-------------------------------------------------------------------------------

>>  Enter your choice: 5

> A logfile (aRMSD_logfile.out) has been written successfully!

-------------------------------------------------------------------------------
<built-in method center of str object at 0x7f7ba4445240> =
-------------------------------------------------------------------------------
-10 Exit aRMSD
-8  Plot aRMSD color map
-7  Change general RMSD settings
-6  Add/remove bond
-4  Change plot settings
-3  Define two substructures (structures are defined: 'False')
-2  Change weighting function
-1  Perform Kabsch alignment (required for all functions)
-------------------------------------------------------------------------------
    Current weighting function  : 'none'
    Calculate mcc contribution  : 'False'
    Kabsch alignment performed  : 'True'
-------------------------------------------------------------------------------
0   ... visualize results in aRMSD representation
1   ... visualize structural superposition
2   ... perform statistic investigation of bond lengths and angles
3   ... show RMSD results
4   ... interpolate between the structures (cart., 10 steps)
5   ... generate outfile
20  ... export structural data
-------------------------------------------------------------------------------

>>  Enter your choice: -10

-------------------------------------------------------------------------------
========================== Normal program termination ==========================
-------------------------------------------------------------------------------
```

◇