

refmac 5.5 bug removal and new features

5.5.105

- 1) A problem related with wrong initial geometry for stats for baubles during TLS and individual atomic refinement has been sorted out (thanks to Eleanor Dodson and Norman Stein)
- 2) Wrong number of the observation introduced recently (I think in v5.5.0104) for twin with intensities has been sorted out. It would cause failure in some cases. (thanks to Norman Stein and Justin)
- 3) Now reading tls parameters that are more than 100 has been sorted out (thanks to Martyn Winn and Ethan Merritt)

5.5.104

- 1) Problem with mixed refinement has been fixed
- 2) Problem with idealisation with the version compiled with bounds check has been fixed (thanks to Norman Stein)
- 3) A problem related with resolution limits for twinned refinement has been fixed (thanks to Norman Stein)

5.5.102

When target angle is 180 then there was a problem especially when electron density was very weak. Fixed.

5.5.0100

A newly introduced problem that would not write out PHCOMB if PHOUT keyword is not defined has been fixed.

5.5.0099

In cases of twin if the program first decided that there are many twin operators (e.g. four) and later removed some of these operators (e.g. the number of remaining twin domains is two) then highest resolution was not always correct. It was related with the fact the the resolution the program works with is the highest resolution after applying all twin operators. If twin is not merohedral then this resolution may be different from actual resolution of the data. This bug has now been fixed.

5.5.0098

Added PHOUT option: outputs the "best" combined phases as PHCOMB and HLiCOMB, $i=\{A,B,C,D\}$

Several less severe bugs found by Norman have been fixed

5.5.0096

A small bug causing segmentation fault in cases of new ligands in refmac has been removed

5.5.0095

A bug related with cubic space group has been fixed. In some cases cubic space refinement would not work because the maximum indices were determined incorrectly.

5.5.0094

The problem related with too many anomalous atoms that caused memory leakage has been temporarily resolved. As a result of this bug file names would change and the program would report unrelated messages like: "Zero length string passed to getenv"

5.5.0092

A problem related with TLS has been fixed. The problem was that not in all cycle TLS contributions were added to B values and that could make refinement unstable.

5.5.0091

A problem related with free R in case of twinning has been sorted out

5.5.0090

A problem with segmentation fault on linux boxes when twin symmetry was inexact has been solved.

5.5.0088

- 1) There were problems when there were more than two datasets in mtz file with very different unit cells. The program would confuse limits in reciprocal space. It has now been fixed.
- 2) IF input TLS were not positive definite the program had problems. Now it has been fixed.

5.5.0082

A problem related with anisotropic scaling in twin refinement is removed. It affected cases when there is no twin.

5.5.0080

Problem related with datasets has been sorted out. In the previous version if there were many datasets in the mtz file then reftmac would take one of them that may have not been related to the column names used in refinement.

5.5.0074

TLS line minimization problem fixed.

5.5.0073

Wavelength reading from mtz header fixed

5.5.0072

If free R was not set then twinning had a problem. It is now fixed

5.5.0071

The problem related with output amplitudes of de-convoluted observations is fixed. In the previous versions not all "observations" were written to the output mtz file. It had no effect on refinement or map calculations.

5.5.0070

Problems related with vdw radii has been fixed. Now non-bonding contacts should work a bit better

5.5.0068

The map coefficients are now calculated using expected values of phase from SAD function (instead of current phases).

An mtz wavelength reading bug fixed.

Crash caused by use of unallocated memory possibly occurring in rare cases fixed.

Crash caused by use of unallocated memory introduced in 5.5.0066 fixed.

5.5.0066

A problem of negative eigenvalues of SAD covariance matrix causing instabilities in SAD Luzzati parameters refinement fixed

5.5.0063

1. Several problems related with size mismatch between subroutines have been sorted out. These problems would surface if the program was compiled with explicit bound checking options.
2. Refmac would loose dataset number for labins corresponding to the observations. It has been fixed with a temporary workaround
3. Potential confusion between R3 and H3 has ben dealt with
4. If RNA/DNA phosphate groups had an atom named OP3 then refmac changes it to O3T and works further
5. A potential mismatch between resolution of data and that calculated from indeces has been dealt with
6. Synonyms have been added to the dictionary to deal with atom names of the monomer SAM

5.5.0055

A problem with incorrect likelihood_free value reported has been fixed.

5.5.0053

A problem related with misinterpretation of mode of likelihood has been resolved. (include file anom.fh has been a little bit rearranged)

5.5.0051

A few remaining compatibility issues for Windows were resolved.

5.5.0050

- 1) Bug introduced in 5.5.0047 related with HKLOUT (output file would not be written if labout is not defined) has been removed
- 2) Inconsistency between document and refmac about alt codes in the external distances restraints removed. Now refmac can take ALTE and ALTC. Document is consistent with the program
- 3) More info about external restraints has been added (distance, angle, torsion, plane, chiral, interval restraints can be defined for any pair or triple etc atoms)

5.5.0047

- 1) Several compatibility issues for irix and windows were resolved. Now it should compile on windows, however this website does not have makefiles for windows yet.
- 2) A bug of user output columns not working correctly under certain circumstances has been removed
- 3) A bug related to ANOM MAPOnly use possibly leading to crash has been fixed
- 4) Refmac can output F+,F-,SIGF+,SIGF- to the output mtz file optionally: those of these that appear in both LABI and LABO will appear in output mtz

5.5.0046

Now unobserved reflections in the output mtz file also have free R flag (equal to zero). It should make programs using this output file happier

5.5.0045

- 1) Ligands con, com, prn were broken. Now they should be ok.
- 2) Added a keyword: weight auto adjust <yes|no > If the value is yes then weight will be adjusted to make sure that rmsbonds are around 0.02 or so. 'yes' is default value.

5.5.0044

- 1) Now the program can read intensities only (i.e. if sigmas for intensities are not available they may not be defined). This option should be avoided. However for some cases from pdb only intensities are available. This option has been added to deal with such cases.
Line minimisation temporary disabled

5.5.0043

- 1) A bug related with FAN and DELFAN maps has been removed. Now the program produces anomalous and different anomalous maps if requested (ANOM MAPOnly) or SAD refinement is performed.
Now refmac with twin refinement prints out all equivalent twin operators. It should help comparing twin laws derived by different programs.
- 2) A keyword allowing refinement of occupancies of anomalous scatterers has been added. If the following keyword: REFIN OREFINE ANOMALOUS then occupancies of anomalous scatterers will be refined
- 3) A keyword added that controls the level of small twin domains. The keyword TWIN FILTERlevel <value> will give a signal to the program that all domains with twin fraction less than given value should be removed. After removal of these domains the program will make sure that twin and crystallographic symmetry operators together form a group. Default value is 0.05

5.5.0042

- 1) A feature has been added: If the keyword ANOM MAPOnly as well F+ and F- have been specified in the labin statement then refmac will produce anomalous difference as well as difference anomalous difference maps. Map coefficients for anomalous difference map are: m DANO_o and m DANO_o - D DANO_c with calculated phase - 90

DANO_o and DANO_c are observed and calculated anomalous differences. m is figure of merit (expected phase error) and D is the maximum likelihood scale parameter that is related with $\langle \cos(2\pi \mathbf{s} \cdot \Delta \mathbf{x}) \rangle$ (expectation value) with \mathbf{s} a reciprocal space vector $\Delta \mathbf{x}$ is error in positional parameters

These map coefficients are calculated by default if SAD refinement is performed, i.e. (i) F+ and F- have been given, (ii) coordinate file contains anomalous scatterers and (iii) wavelength (either in mtz file or using ANOM wave keyword) or ANOM FORM f' f'' statements have been defined.

2) TLS refinement has been stabilised further

3) If keyword TLSO ADDU keyword is given then the program output coordinate file will contain anisotropic U values calculated from TLS parameters and isotropic equivalent of TLS contribution will be added to B values. At this stage this keyword should be used for visualisation and analysis purposes. Output file thus produced should not be used in the next stage of refinement

4) Bugs related with premature termination of refinement has been removed

5.5.0040

An introduced bug affecting SAD refinement has been removed

5.5.0039

A bug related with the high B values of non-tls groups has been removed

Automatic definition of domains as segments or chains sometimes had some problem

Stability of the multidimensional integration to derive the posterior expectation values for twin and intensity based maximum likelihood refinement has been improved

5.5.0038

Bug related with addition of non-tls group to one of the groups has been removed

5.5.0037

If auto weighting is specified (note that it is default) then the program will try to make sure that zbond is between 0.2 and 1.0.

If the input pdb file had anisou card and isotropic refinement is performed then the output file contained anisou card with only the first element non-zero

Refinement exits if function value starts to increase.

Inaccuracy in mask based solvent contribution calculations has been corrected. Now R/Rfree should look better.

If ligands are close to one of the tls groups they are not included in these groups. Only metals and solvent molecules are added to TLS groups. Note that it is users' responsibility to make sure that all atoms in the asymmetric unit belong to one or another tls group.

5.5.0036

For some groups small twin domains were not removed correctly. Now they are removed correctly. The program makes sure that space group symmetry together with twin symmetry form a group

An option added not to add waters to tls groups. New keyword is: tlsdetails waters exclude
A little bit better option for autoweighting

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