Version 29/08/2025 build 2.1:

Previous versions used the TMP subdirectory in the Jana2020 home directory for temporary, working files. In addition, initialization and history files are also placed in the Jana2020 home directory. It led to the condition that the user must have read/write/delete access to that directory. This condition was not possible when the program is installed centrally, and writing to the installation directory is blocked. The new version uses the Jana2020 subdirectory created in the C:\Users\<username>\AppData\Roaming. When installing a new version, the content of these files is copied to the new location for older users.

Wyckoff symbols – The procedure for editing atoms shows the Wyckoff symbols together with the site symmetry and multiplicity.
CIF dictionary – The dictionary for electron diffraction data and modulated structures has been updated.
PwdLib, JanaLib – The instrumental resolution function (extension "irf") used for TOF data can now be exported as a standard.
PwdLib – Several improvements in the reading "irf" have been made.
JanaLib – The initialization file Jana2020.ini and the CIF file created for the structure ("structure_name" .cif) can be directly edited from the command tree.
SIR, Expo – The revision and correction of how different versions of these programs are called has been made.
Editm50 – For magnetic structures, the symmetry dialog has been changed to allow the half shift in x4, x5, and x6 of the magnetic inversion operator to be inserted explicitly.
JanaLib – The space group symbol has supplemented the status bar information.
Refine – For multi-pole refinement, automatic blocking of the kappa' parameter has been added if all asymmetry parameters are zero.

Version 17/07/2025 build 1.3.62:

Modification of the CIF dictionary – The new dictionary for modulated structures and structures determined from electron diffraction data was modified by the kinematical and dynamical approach. For the modulated structures, most ad hoc terms '_Jana_' were replaced by official ones. However, the new version read both new and old CIF files.
JanaDraw, GraphT – Extended the capabilities of calling GraphT after selecting atoms in JanaDraw.
Refine – Correction of the calculation derivatives for magnetic structure factors, refined against single crystal data, considerably speeding up the refinement process.
Refine – The neutrality condition was corrected so that the total number of valence electrons equals the difference between the number of protons and core electrons.
Refine – An error occurred when combining the scaling parameters in the equations entered by the user for the individual zones of electron diffraction data. The derivatives of these parameters were not fully calculated at the right moment.
Refine – The stability of the refinement process has been improved. The program stops refining the most refined parameters with information about the parameters responsible for that issue. The older versions usually crashed without any information.
Manual culling - Added the ability to make reflections visible by group color, or to exclude these reflections from the image. This allows easier detection of systematic errors.

EditM9, PwdLib – Deeper changes related to importing data from WISH. Improved the input of an IRF file individually and introduced the possibility of using a file containing information about all data blocks instead of individual IRF files in the input.
CrystLib – Fixed the calculation of the metric tensor for modulated structures of higher dimensions (3+2) and (3+3). It especially affected drawing de Wolff's sections.
CrystLib – The import of the multipole parameters now uses the new database.
CrystLib – The procedure for finding rational parts of modulation vectors was generalized to higher dimensions (3+2) and (3+3).
CrystLib – The procedure for finding modulation vectors from powder data has been significantly improved.
RepAnalysis – The final information about the possibility of choosing a transformation when creating a current model from the parent structure has been extended to simplify the choice for the user.
Contour, JanaDraw – The calculation and imaging of p.d.f. and j.p.d.f. has been extended to modulated structures.

Version 24/02/2025 build 1.3.61:

Refine – The check of refined structure parameters has been added. Now, if the actual parameter leads to a strongly unrealistic value during the refinement, it gives a message, and the value returns to that from the previous refinement step.
Refine - The R-factor output is now calculated separately for the main and satellite reflections, even for cases when some reflections have both contributions.
General feature – New variables were introduced to specify whether a given atom will be considered a donor and acceptor for hydrogen bonding.
JanaDraw – The limit for the isosurface value is now calculated from the error map error.
CrystLib, EditM9 – The procedure for importing a CIF file created by SHELX and OLEX programs has been improved and completed with newly used data formats.
JanaDraw – Improved procedure for restriction of water molecule geometry.
Refine – Refining the magnetic structure in the F^2 minimization mode led to a very slow convergence. The calculation of derivatives for this case has been corrected.
Refine – The possibility of excluding reflections from refinement based on the current value of the effective wavelength of reflection measured on a single crystal by the TOF method has been implemented.
Refine – At very high Uiso values, an error was reported in cases of enormously large Uiso. This led to an abort of the computation with the erroneous identification of a particular reflection. Newly, the calculation runs without interruption, and the contribution of the relevant atoms is set to zero.
Fourier – During the Fourier summation, the error map value is determined. This is then available for searching for new atoms and drawing a map.
JanaDraw – Map drawing for (3+2)d modulated structures has been added.
JanaDraw – Added an indication that some atomic types have been filtered out to the bottom toolbar. The same is done when removing links from the image.
JanaDraw – Added parameter to enlarge the displayed map by the of atomic radii.
General feature – The program has been modified to use newly introduced parameters to correct anisotropic incoherent mozaicity.
General feature – The program goes automatically to the import wizard if it is called from the file with the extension "cif_pets."

Editm50 – A space group test by calling SGTest program written by Stokes & Campbell is now possible for all cases.

Version 27/10/2024 build 1.3.60:

General feature: How the so-called rejected atoms, which means the atom for which the ADP Uiso parameter goes above the chosen limit, are handled has been modified. These atoms can now be deleted from the item "Edit structural parameter" of the command tree.

General feature: The status line with structure information summary has been modified to give more information, including the number of rejected atoms. Moreover, it is now active on all types of focus (Basic, JanaDraw, and Profile Viewer).

New molecular position: The procedure for introducing a new molecular position under the JanaDraw focus allows the use of the atoms that belong to the previously defined position of the same molecule.

Many other fixes that resolved issues with intermittent bugs have been implemented.

Version 27/10/2024 build 1.3.58:

JanaDraw: The figure can now be combined with the Fourier, density, and j.p.d.f. maps.

Refine: A new possibility of using individual weighting for individual data blocks of joint refinement has been introduced.

Refine: Two new R factors were introduced for magnetic structure for cases when the diffraction spot is composed of magnetic and nuclear contributions.

Contour: The mouse can introduce a new crenel function from the DeWolff map.

Contour: The procedure for transforming x4-maps to t-maps works now faster (OpenMP).

Contour: The procedure for calculating maps in a general section now works faster (OpenMP).

General: The origin definition for non-standard space and superspace groups having an X-centering symbol was introduced. The problems or ambiguities were solved.

SuperFlip: The default parameters have been modified based on experience using this procedure.

General: The testing procedure for absolute configuration has been included.

Import/reimport data from Pets: The procedure for importing data from Pets now checks if data was created for kinematical or dynamical refinement. The same procedure is also called when, during the editing, we ask for switching from kinematical to dynamical refinement or vice versa.

Data import: The process has been modified to improve behavior when reimporting data.

Dynamical refinement for electron diffraction data: The program was modified to allow using a new, improved Dingo program, which allows a more general procedure for thickness correction and a new option for mosaicity.

Fourier: The procedure for peak searching has been considerably improved by the application OpenMP.

Fourier: The default limit for the peak searching is now based on the multiple of the error map value.

General: The possibility of getting a patched exe file was open for users without asking for a password.

Version 19/07/2024 build 1.3.56:

Importing Pets file: A crash occurred when the new structure was created from the cif_pets file in the previous version.

Contour: The process for creating p.d.f. and j.p.d.f. Maps have been modified. Now, it works faster.

Transformation: The procedure for transforming from the commensurate to supercell description has been corrected. In the old version, the atoms merging process did not work correctly for some specific cases.

Magnetic modes: Several issues were corrected.

Cyclic refinement: The procedure has been generalized for the GSAS data containing several banks in one data file.

Representation analysis: The old version could read the new CIF files from ISODISTORT.

Version 19/07/2024 build 1.3.55

Contour+JanaDraw: The procedure for systematic search for critical points of the electron density map calculated based on the results of multipole refinement has been significantly improved. Critical points can be displayed directly in the JanaDraw program.

Symmetry check of modulation vectors: The procedure for checking the consistency of modulation vectors with selected symmetry has been modified to work for general cases of (3+2)d and (3+3)d of a modulated structure. Previous versions pointed out the disagreement, although the differences were negligible.

Distance calculation: The procedure for calculating the best planes through selected atoms ignored atomic names containing a symmetry code.

Sorting satellite reflections: During the reflection merging procedure, the information in the output did not include all satellite reflection groups. This only concerns (3+2)d and (3+3)d modulated structures.

Completing of the structure with hydrogen atoms: In the JanaDraw graphics program, the possibility of adding hydrogen atoms has been newly introduced, even if the non-hydrogen atoms were not exclusively part of an atomic or molecular block. After adding hydrogen atoms, the selected geometric conditions are activated and applied during the refinement.

Localization of maxima in the map: This process became very lengthy for the case of (3+2)d and (3+3)d modulated structures. The application of multiprocessor sharing has greatly accelerated this process.

Drawing graphs by modulating parameters (GraphT): The old program version went into a dead state when drawing angles from one selected atom of the neighbors between atoms or BVS values when choosing a distance too short to detect any neighbor. A warning will now appear, and the user can select a different limit value.

JanaDraw: The previous version allowed displaying Fourier, p.d.f. and j.p.d.f. maps and de Wolff sections after selecting a region defined by one or more atoms. The new version allows the same for electron density maps based on multpole refinement.

Version 19/06/2024 build 1.3.54 :

Jana2020→Superflip: The pattern-matching procedure option has been enabled for powder samples. To this end, the relevant dialogue has been modified.

Make CIF: The CIF file creation procedure has been modified to output the weighting scheme used. An analogous method to the one used by SHELX was used, which reduces the problems of checking with CheckCIF.

Cyclic refinement: The procedure has been extended to cases where the data comprises several banks.

Cyclic refinement: The option to display powder profiles in a single graph was added.

Copy in, save as: These functions did not work correctly for cases where the crystal is composed of multiple phases when using the JanaDraw procedure. The same was true for composite structures.

Make refinement reflection file: The option to run this procedure in silent mode has been created.

Data import: The data input in the FullProf format for single crystals has been modified to respect the differences between TOF data and CW data.

Dist+JanaDraw: The new version does not automatically draw or calculate distances and angles between atoms described as different positions of the same molecule.

Making continuous motifs: The procedure is based on atomic radii instead of the previously used typical distances. This reduces problems in the case of incorrectly determined atomic types when solving the structure.

New molecular positions from JanaDraw: The procedure has been modified to simplify the work in the case of many overlapping molecules caused by a disorder.

Refinement: The ability to fix the shape of water molecules has been added to geometric keep commands.

Drawing of magnetic moments: In addition to the original drawing of the magnetic moment, in which the centre of the vector and the atom merge, the possibility of drawing the magnetic vector from the centre of the atom has been added.

Import data: The procedure for importing data from the Koala has been modified following the new data format.

Version 19/01/2024 build 1.3.53 :

Contour: The "fill map with atoms" command can now be used for De Wolff sections too.

Crystlib: The import process of the matrix calculator has been revised to fix various bugs.

Crystlib: You can customize the typical distances and turn them on or off.

EditM9: There have been significant changes to the import procedure. It now provides complete information on the relationship between actual, reference, and reference-derived cell parameters and modulation vectors.

Grapht: The graphical user interface (GUI) dialog has been updated to make it more user-friendly and intuitive.

JanaDraw: The feature to visualize only the existing t-sections for commensurate structures has been added.

JanaDraw: A new feature has been added which allows users to show composite structures on the display.

JanaIndex: The procedure for finding and including reticular twins has been established.

Version 11/08/2023 build 1.3.51 :

Dynamic refinement of electron diffraction data: The new version of the Jana2020 program has been modified to work with the new version of Dyngo, in which Lukáš Palatinus has substantially improved the algorithm for including dynamic diffraction effects.

Crystlib: The new scale factor in the transformation from a commensurable description of the modulated structure to the supercell did not respect the change in cell centration.

Crystlib: The CIF dictionary for loading and producing CIF files has been supplemented with keywords for multipole refinement.

Crystlib: The procedure exporting tables for publications now includes also magnetic parameters.

Editm9: Importing "pets" files in some cases incorrectly read the orientation matrix.

EditM40: The option for adding hydrogen atoms from JanaDraw by manual selection of the central atom and its neighbours from the figure, has been improved.

EditM40: A new interaction procedure has been added that allows the sorting of atoms on an M40 file.

JanaDraw: Defining restrains of distances, angles, and torsional angles from JanaDraw has been completed with all options allowed in the refinement program. In the previous version, this was accessible only from the procedure for defining refinement commands.

Version 09/07/2023 build 1.3.50 :

Basic Jana window: The status line of the Basic window was supplemented with information about whether a wizard, le Bail, or Rietveld procedure is in progress. In addition, for cases where the process takes place in several steps, the right part of the basic Jana window indicates what stage we are currently in and what will follow in the next steps.

JanaDraw: In the previous version, the possibility to enter a new position of the molecule directly from the image was accidentally eliminated.

Refine: The interpretation of the profile parameters will now be made for all phases present in the sample.

Refine: Multipole refinement for data measured by electron diffraction led to divergence in the application of electroneutrality. This error is caused by a faulty application of the Mott formula.

Refine: The extinction correction has been modified to work better for cases of extremely strong extinction effects.

Refine: The use of a general matrix for a supercell has been extended to the commensurably modulated structures (3+2)d and (3+3)d.

Profile viewer: Added the ability to display advanced background functionality.

Profile viewer: The specification of parameters describing the profile has been improved. This is particularly evident in the specification of profile parameters using the le Bail method in cases where there is a strong overlap of diffraction traces.

Solution by SIR-ware programs: In some special cases, importing results from the run of these programs did not work correctly.

Random search for modulation vectors: The procedure has been considerably improved.

Data import procedure: The information displayed in the dialog boxes has been modified to better inform users about data import and transformation options.

Data import procedure: The procedure for importing "pets" format data did not respect the original transformation matrix of the current cell.

Version 06/04/2023 build 1.3.49 :

Run Superflip: In the previous version of the Jana2020 program, there was a serious error in the preparation of files for the Superflip structure solution from electron data. This error completely blocked this program from starting.

Data import: The procedure for importing magnetic structure data from SXD ISIS has been improved.

Refinement: The possibility of refining of the anomalous corrections f' and f" has been improved.

JanaDraw: The possibility of direct export of the displayed structure to the Diamond drawing program was added.

Version 21/03/2023 build 1.3.48 :

Contour, Fourier: The maps are calculated by default for the whole cell instead of the independent parallelopiped.

Contour: The procedure for recording maps in a movie has been improved.

Contour: The dialog for drawing p.d.f. and j,p,d,f, maps has been improved.

Space group test: The procedure has been modified and improved. The recent version allows making the space group test based on the cell parameters from the data collection or based on the actually used cell, including already introduced twin matrices.

Dist: The bug in the dialog for defining BVS has been corrected.

Data import: The whole procedure has been revised with respect to the possibility of introducing the twin domains already during the data import and taking full information for the cif_od file in the case of importing the hklf5 file.

Manual culling: A new option for exporting an information file in which all reflection intensities before merging are listed together with the averaged and calculated values. This procedure is started only on request from the main Jana menu.

Edit molecules: Several bugs in the dialogs for editing advanced modulated parameters (TLS modulations, molecular crenels) were corrected.

Grapht: The rarely used option for drawing x, y, and z coordinates has been replaced by drawing the displacement from the averaged position.

JanaDraw: A new option to visualize the hydrogen bonds has been included.

JanaDraw: For commensurate cases, the program can now visualize only the existing t, u, v sections of the structure.

JanaDraw: The Grapht can be called directly from the JanaDraw program by using the Grapht mode. It can visualize different parameters depending on made selection.

JanaDraw: The refinement commands to fix or restrict structural parameters can be defined directly from the figure.

JanaDraw: The new geometrical restraints to keep ideal triangular, tetrahedral, and octahedral geometry can be imposed directly from the drawing program.

Simulation of the diffraction pattern: A new option for drawing coexisting cells has been implemented.

Powder refinement: A new option to use the standard profile to interpret the refined profile parameters to get the crystal size and strain has been included.

Powder profile: The zoom behaviour triggered by the mouse wheel has been improved. In older versions, it froze when the minimum window was reached. The return was then only possible with the help of the "Shrink" button.

Refine: The procedure for overlapping of modulated reflections defined by an interval to exclude incompletely overlapped reflections was corrected to work in exactly same way as for overlapping of random twins.

Random search for modulation vector(s): The procedure has been substantially improved. Especially for the case when it is used to find the propagation vectors of a magnetic structure called from a parent structure.

Version 22/12/2022 build 1.3.47 :

Contour: To draw the course of the map along the selected trajectory, the ability to display the derivative curve has been added.

CrystLib: When you create a cif file for publication, you are now offered the option to perform a check with the CheckCIF program. However, this requires online access to the Internet.

CrystLib: The procedure for creating tables for publication has been improved.

Dist: The ability to export hydrogen bond characteristics for modulated structures has been added.

Refine: The newly created 64-bit program Dyngo by Lukáš Palatinus is now associated with the 64-bit version of Jana2020.

JanaDraw: In the mode of entering program refinement commands, it is possible to use the measuring distances, angles and torsional angles to perform their limitations.

Version 21/11/2022 build 1.3.46 :

General: Starting with this version, it will be possible to get individual patches of the current version by using Atl+P in the "About Jana2020" dialog. This will open a password-protected dialog. I will give you the current password based on an individual query.

Contour: In the case of Contour calls from the powder profile viewer, graphics crashed in some cases.

Contour: When entering a new position of an atom from the map, there are sometimes problems with memory allocation.

Structure solution by SHELXT: The new version can run solutions even if it exists in a multi-domain twin structure.

Matrix calculator: Modifications have been made that substantially simplify the import of matrices from the structure.

Data import: In cases where HKLF5 input is used and twinning matrices are known, this information is recorded on the repository file m95.

Cyclic refinement: For crystal structures containing several phases, a number of errors in the graphical presentation of results have been fixed.

JanaDraw: Entering new atoms from the lists of found maxima from difference Fourier maps has been simplified.

JanaDraw: The selection of bonds from the picture proceeded differently from the selection of atoms and illogically.

Magnetic structures: The magnetic structure can be exported to the MVIZUALIZE drawing program on the Bilbao Crystallographic Server by the "Draw structure → Call MVizualize" option.

Jana2020 basic window: Two new features have been implemented – "Rename the structure" and "Transform to the standard setting "

Profile viewer: In some cases, the dialog boxes for X(min) and X(max) did not display the current values.

Refine: For magnetic structures, the program now displays the sum of the magnetic moments of each atom of the structure in the cell and their sum for all atoms of the structure.

Version 06/10/2022 build 1.3.45 :

Data import: The possibility of using another data format from energy dispersion X-ray measurement has been added. The files are characterized by the file extension "npd".

Refine: Added the possibility of using the weight scheme according to the SHLEX program.

JanaDraw: Added parameter defining extensions for filling cell and supercell. In the older version, some atoms lying near the border did not appear.

JanaDraw: The possibility to draw p.d.f.a j.p.d.f. maps directly from JanaDraw has been added.

Version 11/09/2022 build 1.3.44 :

Contour, Manual culling, Grapht, JanaDraw: In the right-side dialog, in addition to the "Tab" key, the "Enter" key can also be used to confirm the change

CrystLib:

1. Fixed incorrect determination of the standard symbol of some superspace groups (SSGs). The error occurred only in cases where the modulation vector contains one or two rational components enforced by symmetry.
2. Determining the direction of the rotational axis of the symmetry operation or the twin matrix always indicated only the nearest crystallographic direction. For the general direction, this led to incorrect conclusions. Similarly, the normal of the plane of symmetry, or the glade plane, was erroneously stated.
3. Fixed behavior of dialogs for entering typical distances and BVS.

To prepare a CIF file:

1. Then standard CIF flag for the Fourier wave definition to describe the modulated structure has been replaced by the standard one. This increases compatibility with ISODISTORT and Bilbao Crystallographic Server.
2. Fixed FCF file preparation for HKLF5 file use case.
3. When you include Jana files, the program requests confirmation of each file.
4. Activated the function of preparing tables for publication from Jana2006.

Manual culling: It is now possible to exclude individual outlier reflections, as follows from comparison between observed and calculated intensities. The procedure then performs a new averaging and only these individual reflections are culled.

Edit atoms: The manual procedure for renaming atoms poorly displayed the current state when switching between individual blocks of atoms.

Powder options: Several errors in the application of spherical harmonic functions to describe the anisotropic spread of reflections caused by the irregular size of crystallites have been eliminated.

Representation analysis: The new version uses matrices for irreducible representations as created by Harold Stokes and Branton Campbell (version 2011).

Version 28/07/2022 build 1.3.43 :

Magnetic option: The maximal dimension for the diffraction indices was changed from 3 to 4 to allow handling of incommensurately modulated structures with higher modulation vectors in the k star.

Magnetic option: The parent structure does not use anymore the reflection file m90. It is always created from the repository m95 file when needed and when the complete information about selecting active modulation vectors is known.

Edit basic parameters: Editing of the symmetry did not generate (3+2)d matrices correctly for commensurate cases.

Refine commands: Keys for excluding reflections from the refinement did not update from the dialog window. A similar problem existed for the maximal satellite index used for checking overlaps in the twin sample.

Edit atoms: Renaming atoms in the "define" page did not work or even led to a crash for the 64-bit version.

Space group test: In some cases, the procedure for detecting the existence of a large more symmetrical cell went into an endless cycle. It appeared only for the 64-bit version.

Version 30/06/2022 build 1.3.42 :

Magnetic option: The representation analysis in Jana2020 has been modified. In the latest version, more than one modulation vector from the star, induced by the symmetry of the parent structure, can be used. Moreover, users can interactively modify the number of active modulation vectors of the star. However, this version's new option is limited to commensurate magnetic structures.

Magnetic option: The magnetic form factors <j0> can be combined with <j2>, <j4> and <j6> in the ration selected by user. For lanthanides, the coefficient of the <j2> term can be calculated from the basic electronic configuration of the actual ion.

You can get detailed descriptions of the new magnetic options on request from Vaclav Petricek.

X-ray form factor problem: The interpolation procedure for the form factors to extremely large $\sin\theta/\lambda$ did not work correctly.

Edit atoms: The button for visualization of the symmetry restrictions did not work correctly for multiphase cases.

Version 30/06/2022 build 1.3.41 :

The 64-bit version has been stabilized, and now it is distributed with the name "Jana2020.exe". However, the 32-bit version, compiled with the classical Lahey compiler, is also accessible but now with the name "Jana2020-32bit.exe". The main reason is that it supplies more detailed information if a runtime error appears. After installation, both icons for both versions should appear on your desktop.

Run SHELXT from Jana: The procedure can now be used even for modulated structures. Then it will supply the solution of the basic structure without transferring the files from (3+d) to 3 dimensions.

Magnetic structures: For magnetic space groups of type I and III refined against single-crystal data, the program calculates additional R values for "nuclear" reflections in which only nuclear contribution is considered. This gives users information on how strongly the magnetic ordering affects reflections with nuclear and magnetic contributions.

TOF data POWGEN: A options for exporting data to the "instprm" file has been included.

Version 21/05/2022 build 1.3.40

64bit Jana2020 version: The latest Lahey-GNU compiler was used to make a 64bit version of Jana2020. The exe file is distributed with the name Jana2020-LGF.exe.

magCIF: Old version did not correctly divide the centering and rotation magCIF tags.

Reading of atom names with apostrophe: The problem could appear when the atom name is copied by the copy-paste method from Microsoft Word or other programs which uses symbols such as Acute accent (&#180), left single quotation mark (&#145), and single quotation mark (&#146). The updated version checks it and transforms them to the classical apostrophe (&#39).

CrystLib: The procedure for saving and recalling the symmetry was corrected and improved. This solved several problems when the program switched between commensurate and incommensurate models.

Drawing modulated structures by external program: We returned to the initially used method when the program generates only atoms in the selected part of the space, no matter if the drawing program, such as a Diamond, visualizes the selected border as a cell.

Cyclic refinement: The procedure allows visualization of how distances, angles, and torsion angles change with the cyclic parameter.

Edit of molecular parameters: Several serious bugs were corrected.

Edit of electron diffraction data: The latest version allows group editing of several blocks of data.

Transformation during the data import: For modulated structure the transformation matrix ignored the mixed block.

Fourier: The latest version allows the combination of several blocks of data into one Fourier map. This is especially useful for complicated structures measured by electron diffraction.

Grapht: After calling this procedure from JanaDraw the program did not return the graphic parameters to those used in JanaDraw.

Version 10/04/2022 build 1.3.39

Jana for Superflip and SHELXT: The problem with using the reflection file of the type "hklf5" has been solved.

Powder profile viewer: The handling of the manual background was improved.

TOF powder option: The new parameters needed for POWGEN data were introduced and the whole TOF powder option was revised.

Cyclic refinement: The latest version for single crystal data read the actual cell parameters and their standard uncertainties from the input files.

Cyclic refinement: The new option to draw distances, angles and torsion angles as a function of the cyclic parameter has been added.

Refinement: Updating the figure by calling JanaDraw for commensurately modulated structures did not work correctly.

Refinement + editing of atoms: In the latest version, we can use the parameter defining the site occupancy names for atoms and molecules "occ" and "occmol", respectively. The old names "ai" and "aimol" are still accepted as aliases.

JanaDraw: A new possibility to select atoms of the actual position of the molecules has been included.

Version 07/03/2022 build 1.3.38

Contour: Several bugs in the procedure for the Monte-Carlo simulation of the error map were corrected

Refine + Powder library: The severe bug in the refinement procedure, called from the profile viewer at the regime when d values define the x-axis, has been corrected.

Matrix calculator: The import of twinning matrixes from the selected structure did not work correctly.

Import from SHELX: The information about the used wavelength was not correctly interpreted.

Cyclic refinement: Several bugs were corrected.

Running of zero cycle: The original number of refinement cycles was in some cases overwritten by zero.

JanaDraw: A new option for selecting bonds for the refine restrains was included. The choice of the atoms allows now to apply a common restriction to all bonds between the selected atoms.

Reciprocal space viewer: The output to the ASCII file has been activated.

Version 26/02/2022 build 1.3.37

Edit Basic structural parameters: Defining a general matrix for commensurate structures did not work correctly.

Edit Basic structural parameters: The button for the space group test on the page "Symmetry" was not making any action.

JanaDraw: In the old version, the selection simulated powder and single-crystal data led to severe problems if started from JanaDraw. In the new version, the program automatically closes the graphic visualization first.

JanaDraw: Deleting atoms from the structure by Ctrl+DeleteUnder did not remove the selected atoms from the list. Then the selection of atoms by Ctrl+A or by mouse shows the position of atoms already deleted.

JanaDraw+JanaIndex: Several modifications were made to improve displaying the figures.

Edit atoms: The menu for selecting atom types was not correctly activated. It displayed only empty lines.

Contour+JanaDraw: In the old version, the return from Contour to JanaDraw did not update the graphic parameters. Then the selection of atoms showed incorrect positions of selected rectangles.

Refine + Power library: The new option for TOF data from POWGEN was introduced.

Cyclic refinement: The possibility to use more banks for powder data was implemented.

Cyclic refinement: It can be used even for single crystal data sets.

Grapht: There were several severe bugs in this procedure.

Version 21/01/2022 build 1.3.36

Representation analysis: Several bugs in the testing procedure calling the listing output and powder profile were corrected.

Edit atoms: Fixed errors in the display of significance, $p/\sigma(p)$ of refined parameters.

Refine commands: The program ignored changes when defining the parameter controlling the output of correlations.

Window11 problems: More corrections make to allows running the program under Windows11.

Version 15/01/2022 build 1.3.35

Window11 problems: It turned out that some WINTERACTER library procedure calls led to problems working under Windows11.

Representation analysis: The transformation, as proposed in ISODISTORT, was in some cases incorrectly applied to symmetry operations.

Grapht: Added the ability to use animation of graphs and maps for cases with two or three modulation vectors.

Version 05/01/2022 build 1.3.34

Representation analysis: The ability to choose from defined propagation vectors those that are to be active has been introduced. This allows simple filtration of isotropic groups as they are generated in ISODISTORT.

Solution by SHELX: The possibility to include twin matrices in the result of the structure solution has been added.

New tools: In the new version, it is possible to display the periodic table of elements in the basic window and in the dialogs where the chemical formula is entered.

Space group test: During the space group test, triclinic point groups were misinterpreted in the phase of finding centering vectors.

JanaDraw: The graphical interface has been substantially changed. The possibility to switch between different modes for interactive input of fixed, restrict, keep commands, and bond restraints has been added. Moreover, it was also added mode for adding new molecular positions, has been.

Profile viewer: Several side effects when interacting with the user have been removed.

Version 06/12/2021 build 1.3.33

Le Bail + Rietveld wizard: Both can be now started directly from the basic focus, for the parent and also regular structure.

Space group test: The cell centering test shows the results for each item continuously. For powder samples, for which this part of the test is time consuming, the user gets an immediate overview of the results.

Space group test: Transformation of the test result into the originally selected cell for the modulated structures spoiled the modulation vectors in some cases.

Input reflection data: Misinterpretation of the neutron measurement headers on the BM11 led to a crash.

Main Jana window: The behavior and appearance of the Jana2020 window has been improved.

DeWolff sections: When using de Wolff sections, the program incorrectly interpreted the type of last computed maps.

Powder profile viewer: Powder profile browser behavior has been improved.

Import powder data: Added the ability to add basic information about the used radiation and grid parameters to the header of the input profile file from the powder profile recorded in a free format.

JanaDraw: A procedure was created to store information about the geometric characteristics and names of atoms in the structure image. During this procedure, the location of the image is fixed.

General: The periodic table of elements can be displayed from the main window and also when entering a chemical formula.

Atom site occupancies: Occupancy of the current position of the atom was incorrectly displayed for some magnetic structures in JanaDraw and when editing atoms.

Version 21/11/2021 build 1.3.31+32

Contour: The procedure for preparing input files for VESTA (General section) and XPlor formats were corrected.

Contour: The older version did not skip atoms with zero occupancies.

Refine: A new procedure for the calculation of the zero-cycle was included as a new option. It can be used to check how structural changes modified R-values.

Representation analysis: A new possibility to filter results from ISODISTORT on the base of active modulation vectors was included.

DatRed: The reading of the Fullprof reflection file for single crystal data was corrected.

EditM90: The merging procedure was considerably modified to make it more user-friendly.

CrystLib: The procedure for finding the transformation matrices between two cells was corrected.

CrystLib: The procedure for finding modulation model by the random procedure was corrected.

JanaDraw: The procedure for visualizing Fourier peaks now checks if the saved maps are actual.

Version 26/10/2021 build 1.3.30

Datred: The data entry for single crystals from FullProf has been fixed.

Version 21/10/2021 build 1.3.29

JanaDraw: The selection of atoms and atomic names was poorly displayed on some computers. Adding the option to choose a delay constant has solved this problem.

Version 19/10/2021 build 1.3.28

Refine: Fixation of molecular parameters in refinement in some cases was not performed sufficiently and required special attention of the user.

JanaDraw: Improved displaying of newly generated hydrogen atoms based on assumed geometry.

Version 17/10/2021 build 1.3.27

Representation analysis: The selection of supercells for commensurate magnetic structures has been expanded and unified.

JanaDraw, Contour: A procedure was created for displaying the evaluated maxima from Fourier maps in JanaDraw and Contour. The displayed maxima can be bent as newly detected atoms of the structure.

Version 20/09/2021 build 1.3.26

Data merging: The procedure did not work correctly for twinned commensurately modulated structures.

Local symmetry for molecular blocks: The option did not work correctly for multiphase single crystals.

Version 06/09/2021 build 1.3.25

JanaDraw: The selection of atoms from the figure was modified. Now the right mouse click & drag deletes the previously selected atoms. For adding newly selected atoms to the list of previously selected ones, the right mouse click & drag is to be combined with Ctrl.

JanaDraw: The direct calling the contour program from JanaDraw is now active even if the number of selected atoms is smaller than 3. Then the orientation of 3d sections is the same as in the figure.

Joint refinement: Several bugs were corrected.

Space group test: The procedure did not work correctly for the trigonal symmetry for modulated crystals.

Simulation of powder profile: The program did not take correctly selected wavelength.

Refine: The complementary occupational modulation was generalized for (3+2) and (3+3)d.

Version 30/08/2021 build 1.3.24

JanaDraw: The possibility to change the view of the figure during the t movie was activated.

JanaDraw: A new option to visualize peaks from the Fourier map was created. This also allows the direct introduction of new atoms from the figure.

Data import: Several bugs in the import of data from Koala were fixed.

Manaul culling: The procedure now works also for reticular twins.

Refine: The procedure for the automatic fixing of the origin was improved.

Version 09/08/2021 build 1.3.23

Edit atoms: The procedure for making contiguous motifs was improved. Now it should look also for short distances between the motifs.

Refine: SHELX extinction correction was modified for electron diffraction

History: The history file was not updated for some transformations

JanaIndex: The option for including twins was considerably improved.

Version 30/07/2021 build 1.3.22

JanaDraw: The way how the program is displaying atomic labels was modified.

Version 29/07/2021 build 1.3.21

Contour: The procedure for DeWolff sections can be used not only for atoms but also for point defined by fractional coordinates.

JanaDraw: The peaks from the difference Fourier map can be visualized in the figure and then used to define new atomic positions.

Version 19/07/2021 build 1.3.20

Representation analysis: Several errors corrected.

Version 15/07/2021 build 1.3.18 + 19

Space group test: Correction for cases: "hklf5 import" and "use old twin"

Edit electron diffraction file: The old unlock edit was changed to new one.

Basic structure file m40: The read/write procedure for Fourier peaks and critical points was included into CrystLib.

JanaDraw: The procedure for handing peaks from difference Fourier was created.

Version 28/06/2021 build 1.3.17

Profile viewer: Irregular behavior of the "Details" option was corrected.

Edit profile: The roughness and zeta (Stephens anisotropic broadening) parameters and could not be activated for the refinement.

Powder data import: The import of the free "only I" data file could not handle more data on one line.

Space group test: Considerably modified.

Random procedure for modulation parameters: New version saves more than only one "optimal" solution.

Procedure for the twin search: Applicable also for merohedric twins.

Version 10/06/2021 build 1.3.16

Grapht: The error connected with drawing of the lines or commensurate sections was corrected.

Version 09/06/2021 build 1.3.15

Reading of molecules: Serious error in the reading of molecules corrected. This error was a new just in the previous version

Version 07/06/2021 build 1.3.14

Contour: The procedure for defining visualized atoms in DeWolff sections was improved.

Contour: The new version allows a direct edit of modulation curves.

Profile viewer: The individual powder profiles from the cyclic refinement can be now selected also from the list and edit box.

JanaDraw: The selection of bonds was block from the global selections Ctrl-A and selection by rectangular boxes.

Define a new molecule: The whole procedure was considerably improved.

Global: Severe bugs using the spherical coordinates for a description of magnetic moments in the case of the presence of more than one phase were solved.

Grapht: Allocation problems were solved.

Version 30/04/2021 build 1.3.9

TOF powder: Several significant changes in import and refinement of TOF powder data. Ability to export "prm" file from Jana2020 refinement.

Version 26/04/2021 build 1.3.8

Data import: The initial transformation matrix for cases with more datasets was, in some cases, corrupt.

Magnetic representation: The magnetic wizard for representation analysis did not handle commands "Next", "Back", and "Cancel" correctly.

Fourier commands: The dialog for defining the parameters for Fourier calculation didn't save the key for weighting.

JanaDraw: The selection of atoms for editing from the figure did not distinguish if the selected atoms are from the atomic or molecular part.

TOF powder option: The program didn't handle the "prm" instrumental file correctly.

Powders: The global cutoff is not activated by default to values d(min)=0.5Å and d(max)=20 Å.

Refinement: The message about the singularity is some cases didn't report the refined parameter correctly.

Jana About: Now the check for a new Jana version is now activated.

Version 13/04/2021 build 1.3.7

Call Jana2006 from Jana2020: It work incorrectly for a structure having in its name the point character.

Output CIF with fcf list code equal 3 and 6 was included.

Contour: Defining of the atoms colors in the maps was considerably modified and improved.

Contour: The possibility to save a map movie in the GIF format was implemented.

Powders: The defined global cutoff was not applied in the calculations.

Powders: In the fundamental approach, the option for divergence slit was not correctly interpreted.

Version 13/04/2021 build 1.3.6

Space group test: A serious bug introduced by the change made in the version 1.3.2, was corrected.

Edit atoms: Bug in changes of ADP parameters for a group of atoms having initially different types of ADPs.

Defining space group from the list: The ESC button did not close correctly the popup dialog.

Version 11/04/2021 build 1.3.5

Edit atoms: A bug in the editing of magnetic moments for a group of atoms was corrected.

JanaDraw: The switch on/off coordinate systems in the options was not working correctly.

Files for BayMem: Several bugs were corrected.

Data import: The twin flag from the CIF reflection file was not passed to Jana.

Non-standard space group settings: More non-standard symbols for monoclinic space groups were included.

Version 7/04/2021 build 1.3.4

Edit atoms: A bug in the editing of ADP options for a group of atoms was corrected.

Dist: A numerical problem in the calculation of best planes was corrected.

JanaDraw: A new information line displaying the number of atoms and bonds was introduced.

Run Superflip: For the solution of the structures having point group 1 or -1, the default option "bestdensities 1 symmetry" was changed to "bestdensities 1 rvalue".

Charge density tools: Several serious bugs were corrected.

Contour: The procedure for the calculation of density maps in the direct space was corrected.

Version 3/04/2021 build 1.3.3

Janalib: The option "Import/modify reflection file" was block for cases when the structure is not yet defined. For importing reflection file, we have to first open and define a new structure or use the new structure wizard.

Contour: Export of maps for modulated structures in the text formats field.

Contour: The drawing of bonds in maps did not worked correctly.

Edit atoms: The possibility to edit a group of atoms has been considerably modified. Now we can change ADPs, modulation parameters, charge density options, and magnetic parameters for all atoms at one time. The locked fields can be unlocked on a request whenever we entered them.

Edit atoms: Editing of multipole parameters crashes in some cases.

Version 1/04/2021 build 1.3.2

Dist: The procedure for calculation of the best plane failed if the number of independent atoms was equal to three. Now it calculates the plane but the refinement step is skipped.

Datred: The procedure that prepares the compressed indices for the diffraction pattern simulation did not consider systematic extinctions which affects simulation figures for twinned structures.

Contour: The procedure for saving maps in the numerical format for (3+d) maps needed to be revised.

Edit atoms: The unlock option was considerably modified. The locking option can also be applied to Radio buttons and Checkboxes. The changes were made to the atom definition of 3d structures, including charge densities.

Version 30/03/2021 build 1.3.1

Grapht: The procedure for adjusting graphs was improved. This was especially crucial for drawing t graphs of interatomic distances.

Edit atoms: The pop-up menu to define atomic types did not work correctly for multiphase samples.

Dated: The procedure for importing data in SHELX format, including the possibility of making absorption correction, did not work correctly for cases when the last diffraction index and the

intensity column had no space for the first ten lines of the file. Now, the test is made in the first 2000 lines.