2020 Canadian Chemical Crystallography Workshop

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Pandemic Edition!!

L12. Crystallographic Information Framework and Validation: The CIF file and checkCIF

Volume 101, Number 3, May–June 1996
Journal of Research of the National Institute of Standards and Technology

[J. Res. Natl. Inst. Stand. Technol. **101**, 341 (1996)]

CIF (Crystallographic Information File): A Standard for Crystallographic Data Interchange

Volume 101 Number 3 May–June 1996

I. D. Brown

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The Crystallographic Information File (CIF) uses the self-defining STAR file structure. This requires the creation of a dictionary of data names and definitions. A basic dictionary of terms needed to describe the crystal structures of small molecules was approved in 1991 and is currently used for become computer interpretable. This offers many possibilities for the automatic handling of crystallographic information.

Key words: crystallographic information; file structures; relational databases; STAR

1. Need for a Crystallographic Information File

Crystallography is rich in numerical information. An x-ray or neutron diffraction pattern of a crystal typically consists of several thousand diffraction peaks, the intensities of which are used to determine the several hundred parameters needed to describe the positions and motions of the atoms. These coordinates are not themselves interesting, but they can be used to calculate the bonding geometry or to display the arrangement of the atoms on a screen. It is therefore convenient to keep the information in an electronically readable form and for this purpose we need a file structure. If the file structure is widely accepted by the community, the information describing the crystal can be readily passed from program to program or from laboratory to laboratory.

Traditionally the results of a scientific investigation are printed in a journal. A crystal structure determination requires that all the atomic coordinates be printed (and, in principle, also the diffraction amplitudes, since they are the primary measurements). The process by which the journal manually typesets extensive tables from a computer listing, and the reader of the journal subsequently keyboards the same numbers back into the computer, is very inefficient and error prone. Recognising this, the International Union of Crystallography (IUCr) decided in 1990 to accept structure reports for *Acta Crystallographica C* in an electronic form generated by the software used for the structure determination. The numerical values in this submission were to be computer checked for consistency and the paper typeset by computer, before the electronic file was passed on to the crystallographic databases for archiving. To facilitate this process the IUCr established the Crystallographic Information File (CIF) as a standard for the transmission of crystallographic data.

Because crystallography, and particularly information technology, are rapidly evolving, it is necessary that the CIF standard also be able to grow. It has to be flexible, allowing for extension as the need arises and, as far as

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Because crystallography, and particularly information technology, are rapidly evolving, it is necessary that the CIF standard also be able to grow. It has to be flexible, allowing for extension as the need arises and, as far as

L12. Crystallographic Information Framework and Validation: The CIF file and checkCIF

First introduced in 1990's as a means of archiving and distributing structural information, as well as a means of formatting and publishing the same structural information (see Acta Crystallographica papers).

Crystal structures are essentially a collection of 3D atomic coordinates (and their ADPs) that define the asymmetric unit, combined with symmetry elements associated with a space group that we use to build the lattice. They are ideally suited to electronic handling and archiving.

Crystal structures are essentially a collection of 3D atomic coordinates that define the asymmetric unit, combined with symmetry elements associated with a space group that we use to build the lattice. They are ideally suited to electronic handling and archiving.

"The crystallographic community needed a common file structure that all crystallographic applications would recognize…the file structure had to be more than just a storage place for archiving the results of crystallographic determinations, it had to be a **crystallographic language** that could be used by computers to explore the wealth of information on crystal chemistry that was even then accumulating in electronic databases." Brown and McMahon, *Acta Cryst.* (2002), **58**, 317-324

What is a CIF?

What is a CIF?

A CIF is simply a text file!

Feel free to edit…

What is a CIF?

The CIF contains the most current information about your crystal (coordinates, ADPs) and the associated refinement data (R-values, residual electron density). It should also contain a complete a copy of the .res file and a list of structure factors. Most refinement packages (Olex2, etc) can generate new .ins and .hkl files directly from the CIF.

The CIF contains fields to be filled in with information about the crystal, its structure, and the refinement results. ShelXL (Crystals? Olex2.refine?) will fill in as many fields related to the refinement as possible, Olex2 (Shelxle? Crystals?) will fill in fields related to the crystal, the X-ray source, diffractometer, etc.

CIFs are generated at the completion of a refinement cycle when the command 'ACTA' is included in your .ins instruction file. In Olex2, if the ACTA tab is selected **a new CIF will overwrite the previous CIF after each cycle**.

What information is found in a CIF?

hi005.cif - Notepad

File Edit Format View Help

```
data_hi005
_audit_creation_date              2020-05-13
_audit_creation_method
;
Olex2 1.3
(compiled 2020.02.04 svn.rd84adfe8 for OlexSys, GUI svn.r6032)
;
_shelx_SHELXL_version_number      '2018/3'
_audit_contact_author_address     ?
_audit_contact_author_email       ?
_audit_contact_author_name        ''
_audit_contact_author_phone       ?
_publ_contact_author_id_orcid     ?
_publ_section_references
;
Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H.
 (2009), J. Appl. Cryst. 42, 339-341.

Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.
;
_chemical_name_common             ?
_chemical_name_systematic         ?
_chemical_formula_moiety          'C25 H19 N O5'
_chemical_formula_sum             'C25 H19 N O5'
_chemical_formula_weight          413.41
_chemical_melting_point           ?
```

Software and versions used to compile the CIF.

Chemical formula input by the user.

What information is found in a CIF?

hi005.cif - Notepad

File Edit Format View Help

```
_space_group_crystal_system         'monoclinic'
_space_group_IT_number              14
_space_group_name_H-M_alt           'P 1 21/n 1'
_space_group_name_Hall              '-P 2yn'
loop_
  _space_group_symop_operation_xyz
 'x, y, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

_cell_length_a                      10.7046(8)
_cell_length_b                      15.0609(11)
_cell_length_c                      12.5922(10)
_cell_angle_alpha                   90
_cell_angle_beta                    99.232(2)
_cell_angle_gamma                   90
_cell_volume                        2003.8(3)
_cell_formula_units_Z               4
_cell_measurement_reflns_used       ?
_cell_measurement_temperature       90(2)
_cell_measurement_theta_max         ?
_cell_measurement_theta_min         ?
```

Information about the space group.

Symmetry equivalent positions as defined by the space group.

Unit cell parameters

What information is found in a CIF?

hi005.cif - Notepad

File Edit Format View Help

```
_space_group_crystal_system         'monoclinic'
_space_group_IT_number              14
_space_group_name_H-M_alt           'P 1 21/n 1'
_space_group_name_Hall              '-P 2yn'
loop_
  _space_group_symop_operation_xyz
 'x, y, z'
 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

_cell_length_a                      10.7046(8)
_cell_length_b                      15.0609(11)
_cell_length_c                      12.5922(10)
_cell_angle_alpha                   90
_cell_angle_beta                    99.232(2)
_cell_angle_gamma                   90
_cell_volume                        2003.8(3)
_cell_formula_units_Z               4
_cell_measurement_reflns_used       ?
_cell_measurement_temperature       90(2)
_cell_measurement_theta_max         ?
_cell_measurement_theta_min         ?
```

Information about the space group.

This (in addition to fractional coordinates) is all that's required to 'build' the crystal.

What information is found in a CIF?

hi005.cif - Notepad

File Edit Format View Help

```
_exptl_crystal_colour                 ?
_exptl_crystal_density_diffrn         1.370
_exptl_crystal_density_meas           ?
_exptl_crystal_density_method         ?
_exptl_crystal_description            ?
_exptl_crystal_F_000                  864
_exptl_crystal_size_max               0.2
_exptl_crystal_size_mid               0.13
_exptl_crystal_size_min               0.09
_exptl_transmission_factor_max        ?
_exptl_transmission_factor_min        ?
_diffrn_reflns_av_R_equivalents       0.0413
_diffrn_reflns_av_unetI/netI          0.0396
_diffrn_reflns_Laue_measured_fraction_full  1.000
_diffrn_reflns_Laue_measured_fraction_max  0.999
_diffrn_reflns_limit_h_max            15
_diffrn_reflns_limit_h_min            -15
_diffrn_reflns_limit_k_max            18
_diffrn_reflns_limit_k_min            -21
_diffrn_reflns_limit_l_max            17
_diffrn_reflns_limit_l_min            -17
_diffrn_reflns_number                 25355
_diffrn_reflns_point_group_measured_fraction_full  1.000
_diffrn_reflns_point_group_measured_fraction_max  0.999
_diffrn_reflns_theta_full             25.242
_diffrn_reflns_theta_max              30.104
_diffrn_reflns_theta_min              2.124
```

Crystal stuff!

Data stuff!

What information is found in a CIF?

hi005.cif - Notepad

File Edit Format View Help

```
 systematic absences.
;
_reflns_threshold_expression       'I > 2\s(I)'
_computing_cell_refinement         ?
_computing_data_collection         ?
_computing_data_reduction          ?
_computing_molecular_graphics      'Olex2 1.3 (Dolomanov et al., 2009)'
_computing_publication_material    'Olex2 1.3 (Dolomanov et al., 2009)'
_computing_structure_refinement    'XL  (Sheldrick, 2008)'
_computing_structure_solution      'SHELXT 2014/5 (Sheldrick, 2014)'
_refine_diff_density_max           0.389
_refine_diff_density_min           -0.271
_refine_diff_density_rms           0.055
_refine_ls_extinction_coef         .
_refine_ls_extinction_method       none
_refine_ls_goodness_of_fit_ref     1.009
_refine_ls_hydrogen_treatment      constr
_refine_ls_matrix_type             full
_refine_ls_number_parameters       282
_refine_ls_number_reflns           5889
_refine_ls_number_restraints       0
_refine_ls_R_factor_all            0.0755
_refine_ls_R_factor_gt             0.0471
_refine_ls_restrained_S_all        1.009
_refine_ls_shift/su_max            0.000
_refine_ls_shift/su_mean           0.000
_refine_ls_structure_factor_coef   Fsqd
_refine_ls_weighting_details
 'w=1/[\s^2^(Fo^2^)+(0.0537P)^2^+0.8469P] where P=(Fo^2^+2Fc^2^)/3'
_refine_ls_weighting_scheme        calc
_refine_ls_wR_factor_gt            0.1066
_refine_ls_wR_factor_ref           0.1202
```

Refinement results!

What information is found in a CIF?

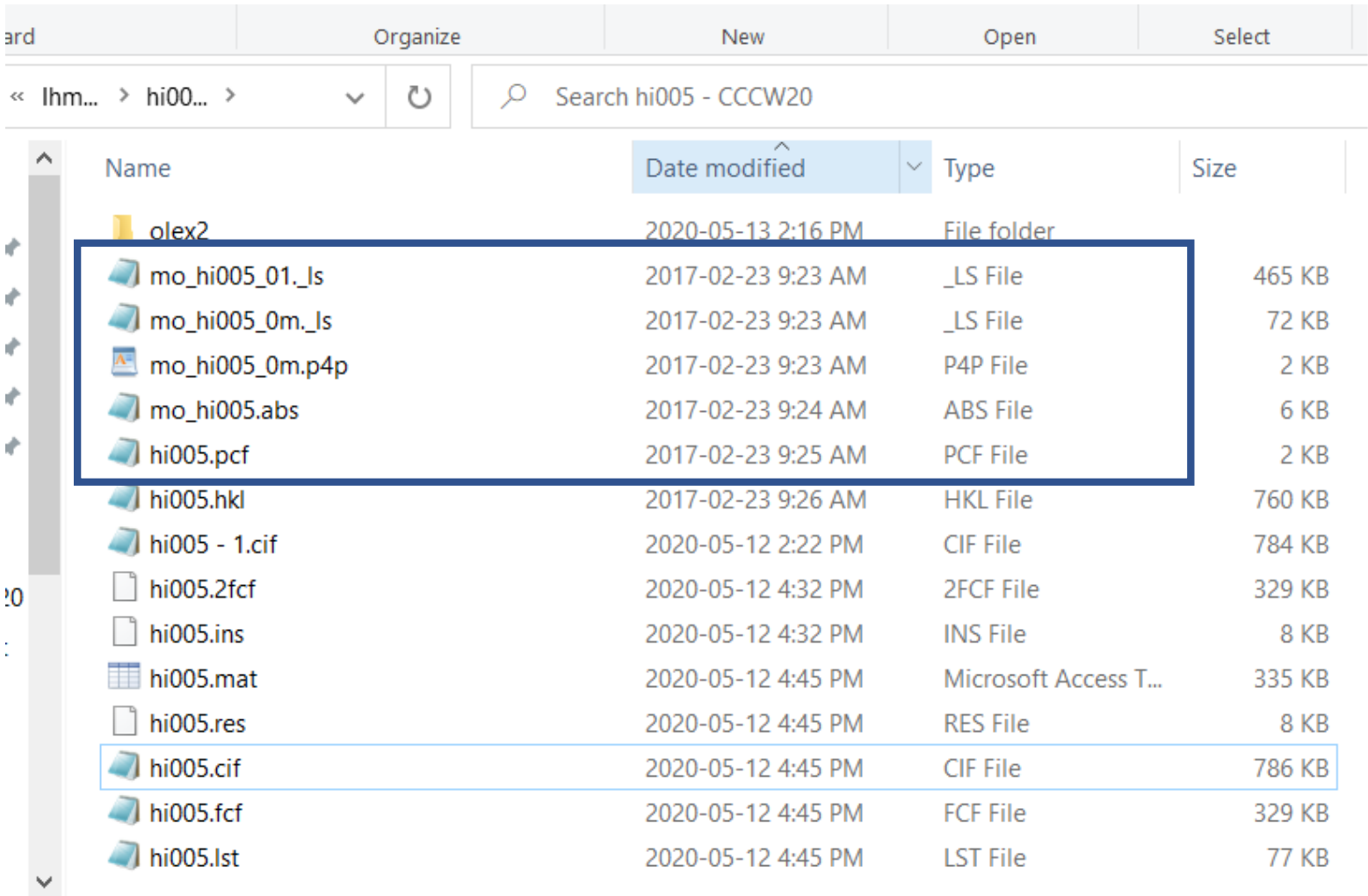
hi005.cif - Notepad

File Edit Format View Help

```
loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_site_symmetry_order
  _atom_site_calc_flag
  _atom_site_refinement_flags_posn
  _atom_site_refinement_flags_adp
  _atom_site_refinement_flags_occupancy
  _atom_site_disorder_assembly
  _atom_site_disorder_group
 C1 C 0.43128(12) 0.30647(9) 0.76383(11) 0.0165(3) Uani 1 1 d . . . . .
 C2 C 0.42198(12) 0.35707(9) 0.66019(11) 0.0156(3) Uani 1 1 d . . . . .
 C3 C 0.36006(13) 0.31957(10) 0.56764(12) 0.0190(3) Uani 1 1 d . . . . .
 H3 H 0.351510 0.256835 0.563392 0.023 Uiso 1 1 calc R U . . .
 C4 C 0.30824(13) 0.37216(11) 0.47773(12) 0.0210(3) Uani 1 1 d . . . . .
 H4 H 0.269297 0.344655 0.412902 0.025 Uiso 1 1 calc R U . . .
 C5 C 0.31474(13) 0.46216(10) 0.48505(11) 0.0185(3) Uani 1 1 d . . . . .
 H5 H 0.274686 0.497927 0.427314 0.022 Uiso 1 1 calc R U . . .
 C6 C 0.38133(12) 0.50238(10) 0.57891(11) 0.0154(3) Uani 1 1 d . . . . .
 C7 C 0.40503(12) 0.59003(9) 0.61100(11) 0.0149(3) Uani 1 1 d . . . . .
 C8 C 0.48317(12) 0.58793(9) 0.71290(11) 0.0138(3) Uani 1 1 d . . . . .
 C9 C 0.50967(12) 0.50118(9) 0.74238(10) 0.0135(3) Uani 1 1 d . . . . .
 C10 C 0.46461(13) 0.21036(10) 0.76275(11) 0.0173(3) Uani 1 1 d . . . . .
 C11 C 0.39778(17) 0.15052(11) 0.81605(16) 0.0317(4) Uani 1 1 d . . . . .
```

Fractional coordinates for each atom! Your structure!

What information is found in a CIF?



What information is found in a CIF?

Without files

hi005 - Copy.cif - Notepad

File Edit Format View Help

```
_exptl_crystal_colour                 ?
_exptl_crystal_density_diffrn         1.370
_exptl_crystal_density_meas           ?
_exptl_crystal_density_method         ?
_exptl_crystal_description            ?
_exptl_crystal_F_000                  864
_exptl_crystal_size_max               0.2
_exptl_crystal_size_mid               0.13
_exptl_crystal_size_min               0.09
_exptl_transmission_factor_max        ?
_exptl_transmission_factor_min        ?
_diffrn_reflns_av_R_equivalents       0.0413
_diffrn_reflns_av_unetI/netI          0.0396
_diffrn_reflns_Laue_measured_fraction_full  1.000
_diffrn_reflns_Laue_measured_fraction_max  0.999
_diffrn_reflns_limit_h_max            15
_diffrn_reflns_limit_h_min            -15
_diffrn_reflns_limit_k_max            18
_diffrn_reflns_limit_k_min            -21
_diffrn_reflns_limit_l_max            17
_diffrn_reflns_limit_l_min            -17
_diffrn_reflns_number                 25355
_diffrn_reflns_point_group_measured_fraction_full  1.000
_diffrn_reflns_point_group_measured_fraction_max  0.999
_diffrn_reflns_theta_full             25.242
_diffrn_reflns_theta_max              30.104
_diffrn_reflns_theta_min              2.124
_diffrn_ambient_temperature           90(2)
_diffrn_detector_area_resol_mean      ?
_diffrn_measured_fraction_theta_full  1.000
_diffrn_measured_fraction_theta_max  0.999
_diffrn_measurement_device_type       ?
_diffrn_measurement_method            ?
_diffrn_radiation_type                MoK\a
_diffrn_radiation_wavelength          0.71073
_diffrn_source                        ?
_reflns_Friedel_coverage              0.000
_reflns_Friedel_fraction_full         .
_reflns_Friedel_fraction_max          .
_reflns_number_gt                     4218
_reflns_number_total                  5889
_reflns_special_details
```

With files

*hi005.cif - Notepad

File Edit Format View Help

```
_exptl_crystal_colour_primary      orange
_exptl_crystal_density_diffrn      1.370
_exptl_crystal_density_meas        ?
_exptl_crystal_density_method      ?
_exptl_crystal_description         'prism'
_exptl_crystal_F_000               864
_exptl_crystal_size_max            0.2
_exptl_crystal_size_mid            0.13
_exptl_crystal_size_min            0.09
_exptl_transmission_factor_max     ?
_exptl_transmission_factor_min     ?
_diffrn_reflns_av_R_equivalents    0.0413
_diffrn_reflns_av_unetI/netI       0.0396
_diffrn_reflns_Laue_measured_fraction_full 1.000
_diffrn_reflns_Laue_measured_fraction_max 0.999
_diffrn_reflns_limit_h_max         15
_diffrn_reflns_limit_h_min         -15
_diffrn_reflns_limit_k_max         18
_diffrn_reflns_limit_k_min         -21
_diffrn_reflns_limit_l_max         17
_diffrn_reflns_limit_l_min         -17
_diffrn_reflns_number              25355
_diffrn_reflns_point_group_measured_fraction_full 1.000
_diffrn_reflns_point_group_measured_fraction_max 0.999
_diffrn_reflns_theta_full          25.242
_diffrn_reflns_theta_max           30.104
_diffrn_reflns_theta_min           2.124
_diffrn_ambient_temperature        90(2)
_diffrn_detector                   'Bruker APEX2 area detector'
_diffrn_detector_area_resol_mean   7.9
_diffrn_detector_type              'CCD area detector'
_diffrn_measured_fraction_theta_full 1.000
_diffrn_measured_fraction_theta_max 0.999
_diffrn_measurement_device         'Bruker D8 Kappa diffractometer'
_diffrn_measurement_device_type    'Bruker APEX II area detector'
_diffrn_measurement_method         '\w and \f scans'
_diffrn_radiation_probe            x-ray
_diffrn_radiation_type             MoK\a
_diffrn_radiation_wavelength       0.71073
_diffrn_source                     'sealed X-ray tube'
_diffrn_source_type                'Incoatec I\ms'
_diffrn_standards_number           0
```

Ln 109, Col 38 | 100% | Windows (CRLF) | UTF-8

Windows (CRLF) | UTF-8

Olex2 will populate fields that describe the crystal, the instrument, etc., from information culled from other Bruker output files.

Structure validation / checkCIF

checkCIF validation ALERTS: what they mean and how to respond

Anthony L. Spek*

The introduction of the CIF standard also opened the way for the automated checking of the archived data for their internal consistency and completeness, which was needed to handle the exploding number of structure reports. The International Union of Crystallography (IUCr) journal *Acta Crystallographica Section C* pioneered automated structure validation as a tool for authors, referees and readers. This

Acta Cryst. (2020). **E76**, 1-11

CheckCIF/Structure validation

Hi Brian,

How are you doing?

I was working on this structure, there is a disordered Phosphorous fragment, I was hoping if you could take a look and help me with the checkcif alerts.
I am attaching the res, cif and checkcif files.

Thank you,

CheckCIF/Structure validation

CheckCIF:

Reads the CIF and performs a myriad of tests (>500!) to assess the validity of the structure. These include, but are not limited to, tests for **missed symmetry**, **missed twinning**, **solvent accessible voids**, and **mis-assigned atom types**.

Accessible via the checkCIF website **(checkcif.iucr.org)** as well as via a stand-alone version available via PLATON.

CheckCIF/Structure validation

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hi005

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Embedded links!!

Datablock: hi005

Bond precision: C-C = 0.0020 A Wavelength=0.71073

Cell: a=10.7046(8) b=15.0609(11) c=12.5922(10)
alpha=90 beta=99.232(2) gamma=90
Temperature: 90 K

	Calculated	Reported
Volume	2003.8(3)	2003.8(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C25 H19 N O5	C25 H19 N O5
Sum formula	C25 H19 N O5	C25 H19 N O5
Mr	413.41	413.41
Dx,g cm-3	1.370	1.370
Z	4	4
Mu (mm-1)	0.096	0.096
F000	864.0	864.0
F000'	864.45	
h,k,lmax	15,21,17	15,21,17
Nref	5895	5889
Tmin,Tmax	0.985,0.991	
Tmin'	0.981	

Correction method= Not given

Data completeness= 0.999 Theta(max)= 30.104

R(reflections)= 0.0471(4218) wR2(reflections)= 0.1202(5889)

CheckCIF/Structure validation

Alert level A

EXPT005_ALERT_1_A _exptl_crystal_description is missing
Crystal habit description.
The following tests will not be performed.
CRYSR_01
DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.
PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used Value .... Please Do !
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value ..... Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value ..... Please Do !
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value ..... Please Do !

Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !

Alert level G

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 5 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.3 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 19 Info

6 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

CheckCIF/Structure validation

Generates "…a report consisting of a list of ALERTS, with associated A, B and C levels of importance, for issues that needed to be addressed. It should be clear the ALERTS are not necessarily errors. They might also point to interesting feature is a crystal structure … All ALERTS should be checked by the authors: a set of lower-level ALERTS may in combination point to a serious issue that needs to be addressed."

While all ALERTS need to be addressed or at least considered, that does not mean that they have to be eliminated (although that is the best outcome). The **Validation Response Form** (vrf) is used to respond to each ALERT.

CheckCIF/Structure validation

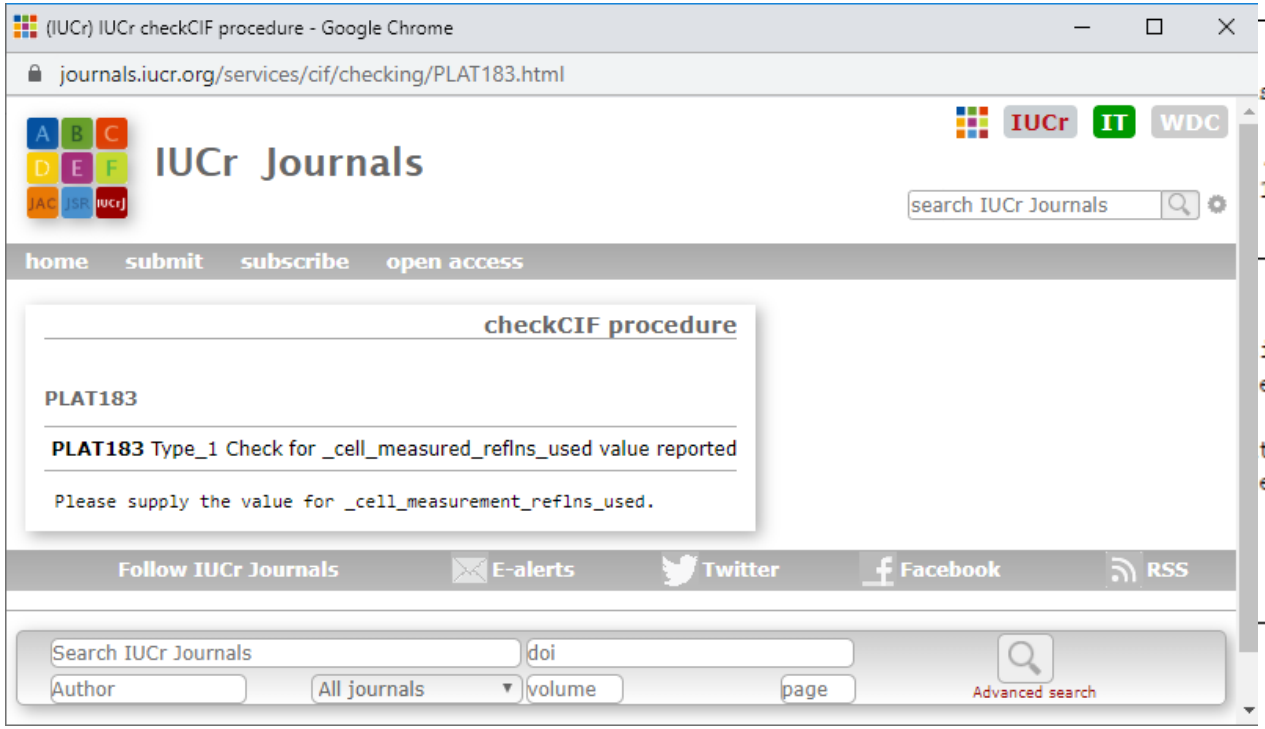
More embedded links!!

Alert level A

EXPT005_ALERT_1_A _exptl_crystal_description is missing
Crystal habit description.
The following tests will not be performed.
CRYSR_01
DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.
PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used Value .... Please Do !
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value ..... Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value ..... Please Do !
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value ..... Please Do !

Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !



Validation Response Forms

CheckCIF/Structure validation

checkCIF

A service of the
International Union of Crystallography

checkCIF reports on the consistency and integrity of crystal structure determinations reported in CIF format.

Please upload your CIF using the form below.

File name:
Choose File jl329.cif

Select form of checkCIF report
- (•) HTML
- ( ) PDF
- ( ) PDF (recommended for CIFs that might take a long time to check)

Select validation type
- (•) Full validation of CIF and structure factors
- ( ) Full IUCr publication validation of CIF and structure factors
- ( ) Validation of CIF only (no structure factors)

Output Validation Response Form
- ( ) Level A alerts only
- (•) Level A and B alerts
- ( ) Level A, B and C alerts
- ( ) None

Send CIF for checking

Information about this version of checkCIF ...

Useful links
Prepublication check for submissions to IUCr journals
Details of checkCIF/PLATON tests
CIF dictionary
Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC

checkCIF is sponsored by

IUCr Journals
CCDC advancing structural science
ACS
ELSEVIER
WILEY
IUCrData
ROYAL SOCIETY OF CHEMISTRY
THE CHEMICAL SOCIETY OF JAPAN NIPPON KAGAKUKAI CSJ
crystals an open access journal by MDPI

CheckCIF/Structure validation

Cut-and-paste the vrf into your CIF, edit in your own response at the '…', save and re-submit to checkCIF.org. **Your new report will include your responses.**

Validation Response Forms

```
  0 ALERT level A = Most likely a serious problem - resolve or explain
  3 ALERT level B = A potentially serious problem, consider carefully
  8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 24 ALERT level G = General information/check it is not something unexpected

  3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 19 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
  6 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_SHFSU01_jl329
;
PROBLEM: The absolute value of parameter shift to su ratio > 0.10
RESPONSE: ...
;
_vrf_PLAT080_jl329
;
PROBLEM: Maximum Shift/Error ..........................       0.16 Why ?
RESPONSE: ...
;
_vrf_PLAT213_jl329
;
PROBLEM: Atom F00P           has ADP max/min Ratio .....        4.8 prolat
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Validation Response Forms

CheckCIF/Structure validation

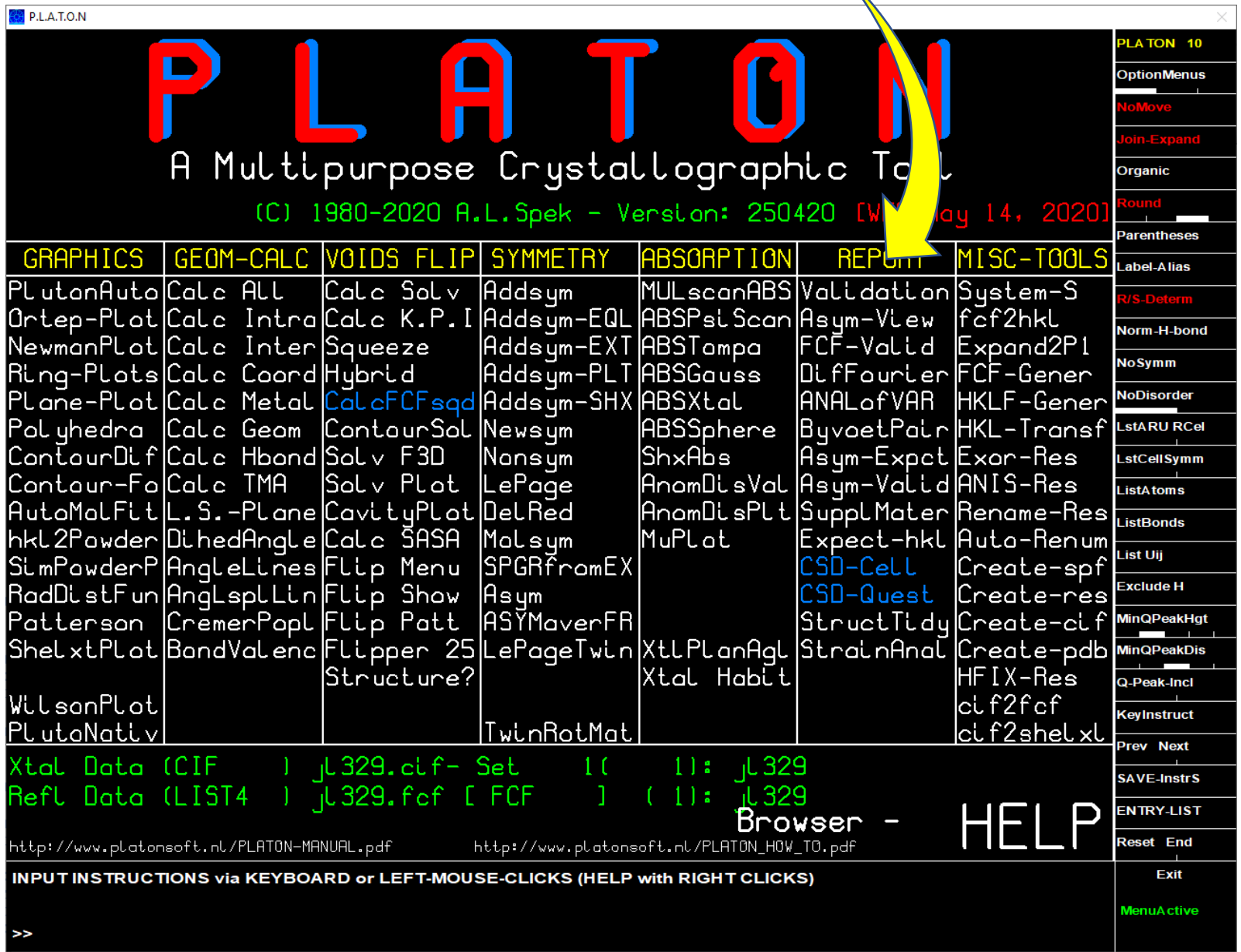
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Validation Response Forms

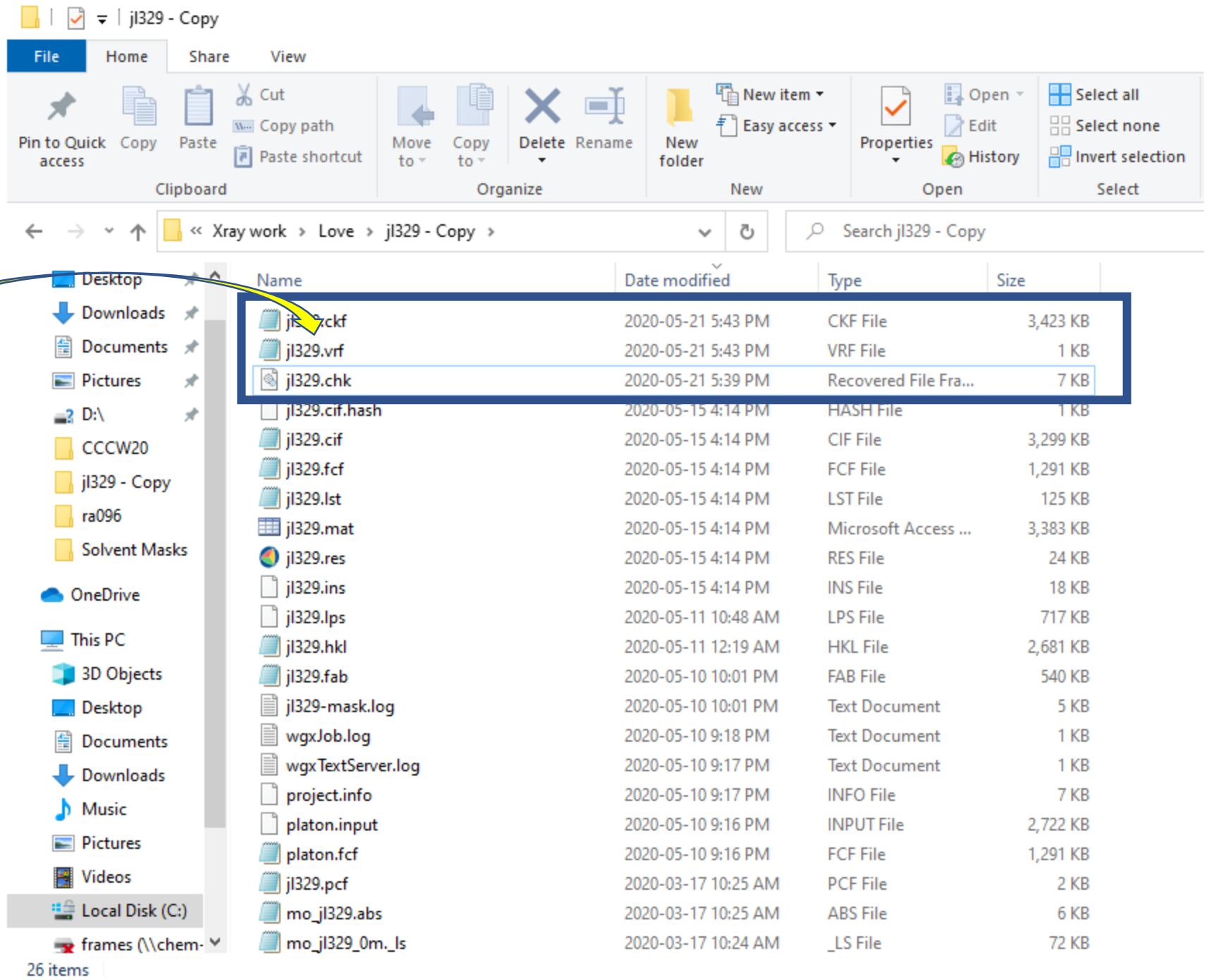
CheckCIF/Structure validation

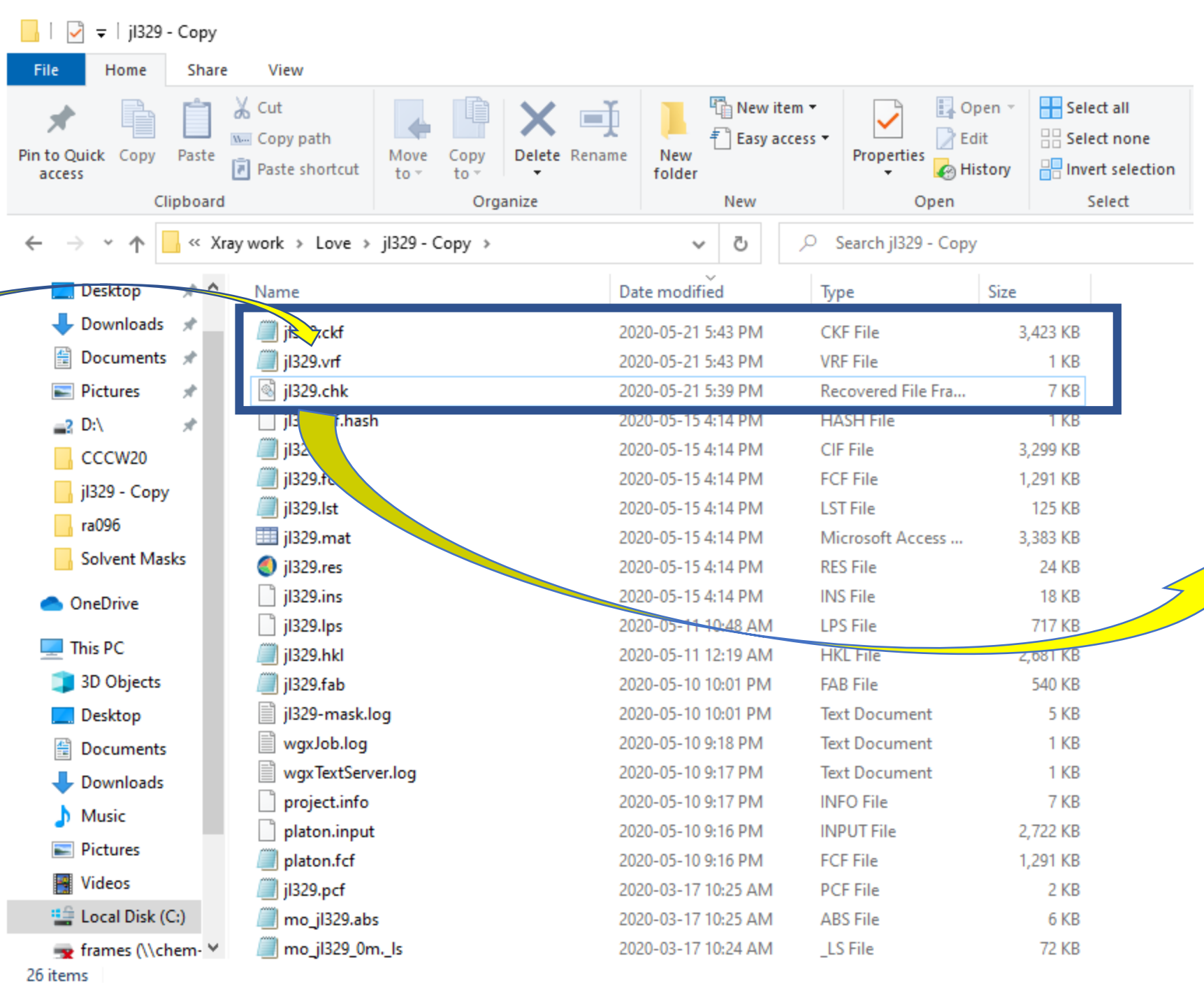
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Can access checkCIF from PLATON directly



Text version of your validation response form





Text version of your validation response form

Text version of your checkCIF report

CheckCIF/Structure validation

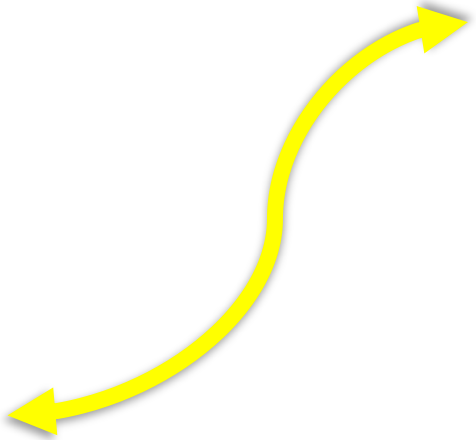
Run checkCIF from PLATON

CifPlus

CheckCIF/Structure validation

CifPlus

Click to edit directly into vrf!



Shape prism Colour orange 0.41 x 0.38 x 0.21 mm^3.

_av_R_equivalents = 0.0452 _av_unetI/netI = 0.0444

Total = 23172 I > 2\s(I) = 16696 Use = 72.1%

MoK\a (λ = 0.71073) T = 90(2) Θ_{max} = 30.523 max/full = 0.999/1.000

SQUEEZE stuff failed!

All U_{eq} < 0.15 All U_{eq} > 0.01

jl329: Rep: C39 H43 Cl F3 N3 Ni | Calc: C39 H43 Cl F3 N3 Ni | C-C = 0.0048

080 ALERT 2 A Maximum Shift/Error ..... 0.45 Why ?

094 ALERT 2 A Ratio of Maximum / Minimum Residual Density .... 9.17 Report

213 ALERT 2 A Atom F00P has ADP max/min Ratio ..... 5.4 prolat

213 ALERT 2 A Atom C1 has ADP max/min Ratio ..... 5.8 prolat

602 ALERT 2 A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

971 ALERT 2 A Check Calcd Resid. Dens. 0.98A From

971 ALERT 2 A Check Calcd Resid. Dens. 0.98A From

971 ALERT 2 A Check Calcd Resid. Dens. 0.98A From

097 ALERT 2 B Large Reported Max. (Positive) Residual Density 4.36 eA-3

934 ALERT 3 B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 10 Check

971 ALERT 2 B Check Calcd Resid. Dens. 0.98A From

971 ALERT 2 B Check Calcd Resid. Dens. 0.98A From

213 ALERT 2 C Atom F1 has ADP max/min Ratio ..... 3.8 prolat

213 ALERT 2 C Atom F00Q has ADP max/min Ratio ..... 3.1 prolat

213 ALERT 2 C Atom F02J has ADP max/min Ratio ..... 3.7 prolat

213 ALERT 2 C Atom F02H has ADP max/min Ratio ..... 3.1 prolat

213 ALERT 2 C Atom F02I has ADP max/min Ratio ..... 3.9 prolat

220 ALERT 2 C NonSolvent Resd 2 C Ueq(max) / Ueq(min) Range 3.9 Ratio

222 ALERT 3 C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 4.1 Ratio

CheckCIF/Structure validation

Validation Response Forms

Shape prism Colour orange 0.41 x 0.38 x 0.21 mm^3.

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213 ALERT 2 A Atom C1 has ADP max/min Ratio ..... 5.8 prolat

602 ALERT 2 A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

Items to be entered into cif file

```
_olex2_diffrn_ambient_temperature_device 'Oxford Cryosystems'
_exptl_crystal_recrystallization_method 'The material was recrystallised from Et2O by s
loop_
  _publ_author_name
  _publ_author_email
  _publ_author_address
  'Love, J.'     ''  'University of British Columbia'
  'Patrick, B.'  ''  'University of British Columbia'

_olex2_submission_original_sample_id WC801
_olex2_exptl_crystal_mounting_method 'The crystal was mounted on a mylar loop in oil'
_publ_contact_author_name          ''


_vrf_PLAT_602_jl329
;PROBLEM: VERY LARGE Solvent Accessible VOID[S] in Structure ! Info:
RESPONSE:
;
```

OK Cancel

CheckCIF/Structure validation

Validation Response Forms

Recorded response remains with CIF throughout.

Common checkCIF ALERTs

Alert level A
PLAT213_ALERT_2_A Atom C39A has ADP max/min Ratio ..... 6.1 prolat

Alert level A
THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5378

Alert level B
PLAT415_ALERT_2_B Short Inter D-H..H-X H47B ..H13B 2.01 Ang.

Alert level B
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low . 0.951 Why?

Alert level B
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 2 Check

Alert level A
PLAT355_ALERT_3_A Long O-H (X0.82,N0.98A) O8 - H7 . 1.15 Ang.