

2023 Canadian Chemical Crystallography Workshop

Crystallographic Information Framework and Validation

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
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I. D. Brown

Brockhouse Institute for Materials
Research, McMaster University,
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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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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.



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“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), B58, 317-324**



Sharon Bellard, David Watson, and Frank Allen,
CCDC Scientists in the 1980s

1987

Allen et al. determine average bond lengths using CSD data

1987

CCDC established as a Registered Charity

1991

Development of CIF format

1992

Relocation to award-winning building





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     ?
_cell_estimated_theta_max       ?
```

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     ?
_cell_measurement_phi_max       ?
_cell_measurement_phi_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  ?
_diffn_reflns_av_R_equivalents 0.0413
_diffn_reflns_av_unetI/netI    0.0396
_diffn_reflns_Laue_measured_fraction_full 1.000
_diffn_reflns_Laue_measured_fraction_max 0.999
_diffn_reflns_limit_h_max      15
_diffn_reflns_limit_h_min      -15
_diffn_reflns_limit_k_max      18
_diffn_reflns_limit_k_min      -21
_diffn_reflns_limit_l_max      17
_diffn_reflns_limit_l_min      -17
_diffn_reflns_number           25355
_diffn_reflns_point_group_measured_fraction_full 1.000
_diffn_reflns_point_group_measured_fraction_max 0.999
_diffn_reflns_theta_full       25.242
_diffn_reflns_theta_max        30.104
_diffn_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
```

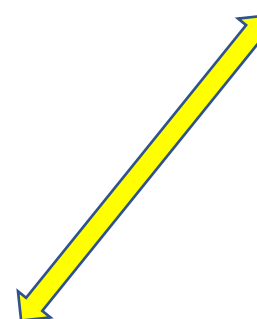
Refinement results!



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?

ard					Organize		New		Open		Select	
<< Ihm... > hi00... >					v		↺		🔍 Search hi005 - CCCW20			
Name					Date modified		Type		Size			
📁 olex2					2020-05-13 2:16 PM		File folder					
📄 mo_hi005_01._ls					2017-02-23 9:23 AM		_LS File		465 KB			
📄 mo_hi005_0m._ls					2017-02-23 9:23 AM		_LS File		72 KB			
📄 mo_hi005_0m.p4p					2017-02-23 9:23 AM		P4P File		2 KB			
📄 mo_hi005.abs					2017-02-23 9:24 AM		ABS File		6 KB			
📄 hi005.pcf					2017-02-23 9:25 AM		PCF File		2 KB			
📄 hi005.hkl					2017-02-23 9:26 AM		HKL File		760 KB			
📄 hi005 - 1.cif					2020-05-12 2:22 PM		CIF File		784 KB			
📄 hi005.2fcf					2020-05-12 4:32 PM		2FCF File		329 KB			
📄 hi005.ins					2020-05-12 4:32 PM		INS File		8 KB			
📄 hi005.mat					2020-05-12 4:45 PM		Microsoft Access T...		335 KB			
📄 hi005.res					2020-05-12 4:45 PM		RES File		8 KB			
📄 hi005.cif					2020-05-12 4:45 PM		CIF File		786 KB			
📄 hi005.fcf					2020-05-12 4:45 PM		FCF File		329 KB			
📄 hi005.lst					2020-05-12 4:45 PM		LST File		77 KB			



Without files

```
hi005 - Copy.cif - Notepad
File Edit Format View Help
_exptl_crystal_colour ?
_exptl_crystal_density_diffn 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 ?
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_diffn_reflns_limit_h_max 15
_diffn_reflns_limit_h_min -15
_diffn_reflns_limit_k_max 18
_diffn_reflns_limit_k_min -21
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_diffn_reflns_point_group_measured_fraction_full 1.000
_diffn_reflns_point_group_measured_fraction_max 0.999
_diffn_reflns_theta_full 25.242
_diffn_reflns_theta_max 30.104
_diffn_reflns_theta_min 2.124
_diffn_ambient_temperature 90(2)
_diffn_detector_area_resol_mean ?
_diffn_measured_fraction_theta_full 1.000
_diffn_measured_fraction_theta_max 0.999
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_diffn_measurement_method ?
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_reflns_number_total 5889
_reflns_special_details
```

What information is found in a CIF?

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File Edit Format View Help
_exptl_crystal_colour_primary orange
_exptl_crystal_density_diffn 1.370
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_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 ?
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_diffn_reflns_av_unetI/netI 0.0396
_diffn_reflns_Laue_measured_fraction_full 1.000
_diffn_reflns_Laue_measured_fraction_max 0.999
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_diffn_reflns_limit_h_min -15
_diffn_reflns_limit_k_max 18
_diffn_reflns_limit_k_min -21
_diffn_reflns_limit_l_max 17
_diffn_reflns_limit_l_min -17
_diffn_reflns_number 25355
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_diffn_reflns_point_group_measured_fraction_max 0.999
_diffn_reflns_theta_full 25.242
_diffn_reflns_theta_max 30.104
_diffn_reflns_theta_min 2.124
_diffn_ambient_temperature 90(2)
_diffn_detector 'Bruker APEX2 area detector'
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_diffn_measured_fraction_theta_max 0.999
_diffn_measurement_device 'Bruker D8 Kappa diffractometer'
_diffn_measurement_device_type 'Bruker APEX II area detector'
_diffn_measurement_method '\w and \f scans'
_diffn_radiation_probe X-ray
_diffn_radiation_type MoK\alpha
_diffn_radiation_wavelength 0.71073
_diffn_source 'sealed X-ray tube'
_diffn_source_type 'Incoatec I\ms'
_diffn_standards_number 0
```

With files

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

Name	Date modified	Type	Size
ALS_BL1131_post_07_2014.cif	2019-03-29 2:59 PM	CIF File	1 KB
ALS_BL1131_pre_07_2014.cif	2019-03-29 2:59 PM	CIF File	1 KB
ALS_Station_11_3_1.cif	2019-03-29 2:59 PM	CIF File	1 KB
apex.cif	2019-03-29 2:59 PM	CIF File	1 KB
archive.def	2019-03-29 2:59 PM	DEF File	1 KB
Bruker APEX2 microsource.cif	2019-03-29 2:59 PM	CIF File	1 KB
Bruker SMART CCD 1K.cif	2019-03-29 2:59 PM	CIF File	1 KB
Bruker SMART CCD 6000.cif	2019-03-29 2:59 PM	CIF File	1 KB
Can_Light_source_BM_XDS.cif	2021-09-22 11:50 AM	CIF File	1 KB
cif_info.def	2019-10-03 4:49 PM	DEF File	3 KB
computing_citations.def	2019-03-29 2:59 PM	DEF File	2 KB
Daresbury SRS station98.cif	2019-03-29 2:59 PM	CIF File	1 KB
DLS_I19.cif	2019-03-29 2:59 PM	CIF File	1 KB
DUO_Cu.cif	2020-01-15 9:55 AM	CIF File	1 KB
DUO_Mo.cif	2015-09-21 4:19 PM	CIF File	1 KB
logo.png	2019-03-29 2:59 PM	PNG File	49 KB
Rigaku R-AXIS Spider.cif	2019-03-29 2:59 PM	CIF File	1 KB
Rigaku AFC12K_724P_007HF_Mo.cif	2019-03-29 2:59 PM	CIF File	2 KB
template.cif	2019-03-29 2:59 PM	CIF File	1 KB
X8.cif	2015-09-21 11:48 AM	CIF File	1 KB

Pna21

C:\Xray work\Schafer\ls964\Pna21.res

C₂₆H₅₆N₇O₂Ta

a = 22.8726(14) **α** = 90° **Z** = 4
b = 11.5384(7) **β** = 90° **Z'** = 1
c = 12.2037(8) **γ** = 90° **V** = 3220.7(4)

R₁ **2.25** %
wR₂ **3.82** %

d min (Mo) **0.76** **I/σ(I)** **29.1** **Rint** **7.01%** **Full 50.5°** **100**
Shift **0.003** **Max Peak** **0.5** **Min Peak** **-0.6** **GooF** **1.009** **Hoof** **.005(5)**

Refinement Finished

Home **Work** **View** **Tools** **Info**

Solve **Refine** **Draw** **Report**

Pna21 **Image** **No Image** **HTML Report**

Style **styles/default.c** **Start** **templates/default** **End** **templates/footer**

Table label style: **As in CIF**

Collection

Crystal

Diffraction

Diffractometer **Bruker APEX-II CCD**

Definition File **C:\Program Files\Olex2-1.5\etc\site\DUO_Mo.cif**

Diffraction T (K) **90(2)**

Cell Measurement T (K) **90(2)**

Special Details **?**

Refine Special Details **?**



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,

Thanks, Brian!

The structure looks a lot better now. I am expecting atleast one of the Oxygen atoms on P to be protonated. As the amine-N is protonated, for charge balance we need one more proton. And just to confirm that there is additional water molecule and not OH-, right?



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/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 Å

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



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

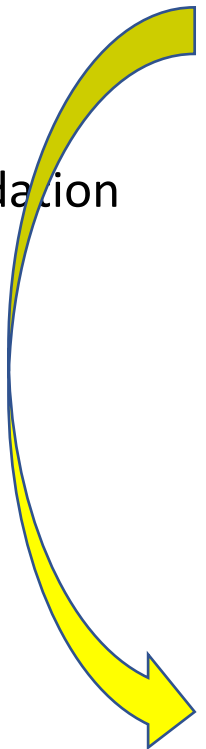
Generates “...a report consisting of a list of ALERTS, with associated A, B and C levels of importance, for issues that needed to be addressed. It should be clear the ALERTS are not necessarily errors. They might also point to interesting feature is a crystal structure ... All ALERTS should be checked 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 !

(IUCr) IUCr checkCIF procedure - Google Chrome

journals.iucr.org/services/cif/checking/PLAT183.html

IUCr Journals

home submit subscribe open access

checkCIF procedure

PLAT183

PLAT183 Type_1 Check for _cell_measured_reflns_used value reported

Please supply the value for _cell_measurement_reflns_used.

Follow IUCr Journals E-alerts Twitter Facebook RSS

Search IUCr Journals doi
Author All journals volume page Advanced search

se Do !
5 Note
.3 Low
19 Info

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Validation Response Forms



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:

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

[Information about this version of checkCIF ...](#)

Useful links

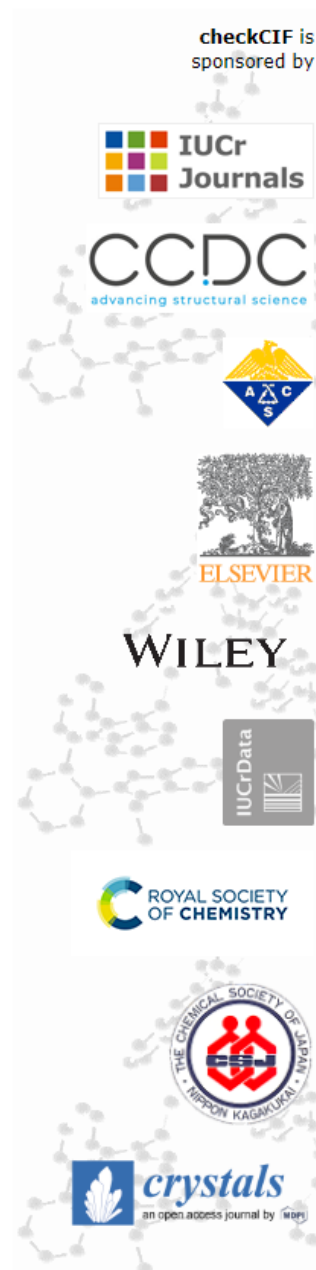
Prepublication check for submissions to IUCr journals

[Details of checkCIF/PLATON tests](#)

[CIF dictionary](#)

[Download CIF editor \(pubCIF\) from the IUCr](#)

[Download CIF editor \(enCIFer\) from the CCDC](#)



CheckCIF/Structure validation



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.

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

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

P.L.A.T.O.N.

PLATON

A Multipurpose Crystallographic Tool

(C) 1980-2020 A.L. Spek - Version: 250420 [W... May 14, 2020]

GRAPHICS	GEOM-CALC	VOIDS FLIP	SYMMETRY	ABSORPTION	REPORT	MISC-TOOLS
PlutonAuto	Calc ALL	Calc Solv	Addsym	MULscanABS	Validation	System-S
Ortep-Plot	Calc Intra	Calc K.P.I	Addsym-EQL	ABSPstScan	Asym-View	fcf2hkl
NewmanPlot	Calc Inter	Squeeze	Addsym-EXT	ABSTampa	FCF-Valid	Expand2Pl
Ring-Plots	Calc Coord	Hybrid	Addsym-PLT	ABSGauss	DiffFourier	FCF-Gener
Plane-Plot	Calc Metal	CalcFCFsqd	Addsym-SHX	ABSxtal	ANALofVAR	HKLF-Gener
Polyhedra	Calc Geom	ContourSol	Newsym	ABSSphere	ByvoetPair	HKL-Transf
ContourDif	Calc Hbond	Solv F3D	Nonsym	ShxAbs	Asym-Expct	Exor-Res
Contour-Fo	Calc TMA	Solv Plot	LePage	AnomDlsVal	Asym-Valid	ANIS-Res
AutoMalFit	L.S.-Plane	CavityPlot	DelRed	AnomDlsPlt	SupplMater	Rename-Res
hkl2Powder	DihedAngle	Calc SASA	Molsym	MuPlot	Expect-hkl	Auto-Renum
SlmPowderP	AngleLines	Flip Menu	SPGRfromEX		CSD-Cell	Create-spf
RadDistFun	AngLsplLin	Flip Show	Asym		CSD-Quest	Create-res
Patterson	CremerPopl	Flip Patt	ASYMaverFR		StructTidy	Create-clf
ShelxtPlot	BondValenc	Flipper 25	LePageTwln	XtlPLanAgl	StrainAnal	Create-pdb
		Structure?		Xtal Habit		HFIX-Res
WilsonPlot						clf2fcf
PlutoNativ			TwlnRotMat			clf2shelxl

Xtal Data (CIF) JL329.cif - Set 1 (1): JL329
 RefL Data (LIST4) JL329.fcf [FCF] (1): JL329

Browser - HELP

http://www.platonsoft.nl/PLATON-MANUAL.pdf http://www.platonsoft.nl/PLATON_HOW_TO.pdf

INPUT INSTRUCTIONS via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)

>>

PLATON 10
 OptionMenus
 NoMove
 Join-Expand
 Organic
 Round
 Parentheses
 Label-Alias
 R/S-Determ
 Norm-H-bond
 NoSymm
 NoDisorder
 ListARU Rcel
 ListCellSymm
 ListAtoms
 ListBonds
 List Uij
 Exclude H
 MinQPeakHgt
 MinQPeakDis
 Q-Peak-Incl
 KeyInstruct
 Prev Next
 SAVE-InstrS
 ENTRY-LIST
 Reset End
 Exit
 MenuActive

Text version of
your validation
response form

File Home Share View

Pin to Quick access Copy Paste Cut Copy path Paste shortcut Move to Copy to Delete Rename New item Easy access Properties Open History Select all Select none Invert selection

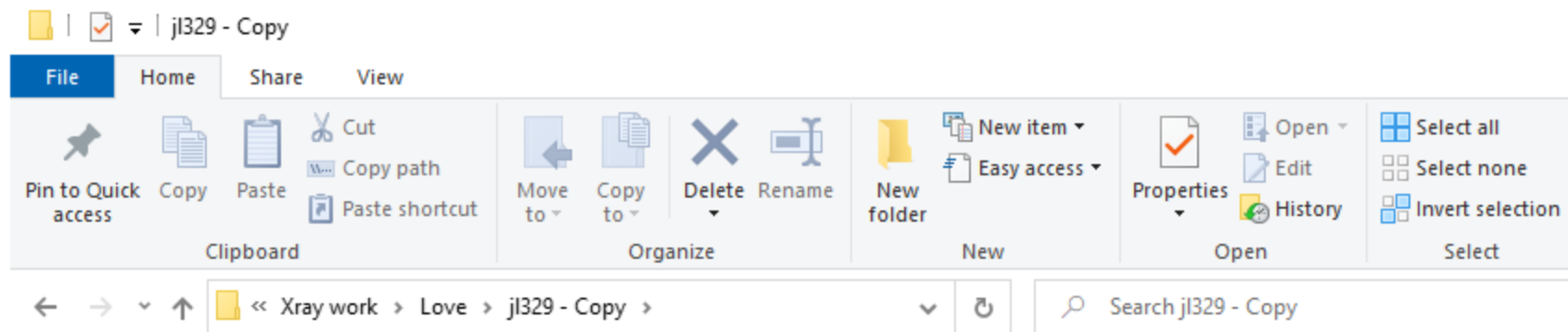
Clipboard Organize New Open Select

Search jl329 - Copy

Desktop Downloads Documents Pictures D:\ CCCW20 jl329 - Copy ra096 Solvent Masks OneDrive This PC 3D Objects Desktop Documents Downloads Music Pictures Videos Local Disk (C:) frames (\\chem-

Name	Date modified	Type	Size
jl329.chk	2020-05-21 5:43 PM	CKF File	3,423 KB
jl329.vrf	2020-05-21 5:43 PM	VRF File	1 KB
jl329.chk	2020-05-21 5:39 PM	Recovered File Fra...	7 KB
jl329.cif.hash	2020-05-15 4:14 PM	HASH File	1 KB
jl329.cif	2020-05-15 4:14 PM	CIF File	3,299 KB
jl329.fcf	2020-05-15 4:14 PM	FCF File	1,291 KB
jl329.lst	2020-05-15 4:14 PM	LST File	125 KB
jl329.mat	2020-05-15 4:14 PM	Microsoft Access ...	3,383 KB
jl329.res	2020-05-15 4:14 PM	RES File	24 KB
jl329.ins	2020-05-15 4:14 PM	INS File	18 KB
jl329.lps	2020-05-11 10:48 AM	LPS File	717 KB
jl329.hkl	2020-05-11 12:19 AM	HKL File	2,681 KB
jl329.fab	2020-05-10 10:01 PM	FAB File	540 KB
jl329-mask.log	2020-05-10 10:01 PM	Text Document	5 KB
wgxJob.log	2020-05-10 9:18 PM	Text Document	1 KB
wgxTextServer.log	2020-05-10 9:17 PM	Text Document	1 KB
project.info	2020-05-10 9:17 PM	INFO File	7 KB
platon.input	2020-05-10 9:16 PM	INPUT File	2,722 KB
platon.fcf	2020-05-10 9:16 PM	FCF File	1,291 KB
jl329.pcf	2020-03-17 10:25 AM	PCF File	2 KB
mo_jl329.abs	2020-03-17 10:25 AM	ABS File	6 KB
mo_jl329_0m_ls	2020-03-17 10:24 AM	_LS File	72 KB

26 items



Text version of
your validation
response form

The screenshot shows the file list in the 'jl329 - Copy' folder. The left sidebar shows the navigation pane with 'Local Disk (C:)' selected. The file list is as follows:

Name	Date modified	Type	Size
jl329.chk	2020-05-21 5:43 PM	CKF File	3,423 KB
jl329.vrf	2020-05-21 5:43 PM	VRF File	1 KB
jl329.chk	2020-05-21 5:39 PM	Recovered File Fra...	7 KB
jl329.f.hash	2020-05-15 4:14 PM	HASH File	1 KB
jl329.cif	2020-05-15 4:14 PM	CIF File	3,299 KB
jl329.fcf	2020-05-15 4:14 PM	FCF File	1,291 KB
jl329.lst	2020-05-15 4:14 PM	LST File	125 KB
jl329.mat	2020-05-15 4:14 PM	Microsoft Access ...	3,383 KB
jl329.res	2020-05-15 4:14 PM	RES File	24 KB
jl329.ins	2020-05-15 4:14 PM	INS File	18 KB
jl329.lps	2020-05-11 10:48 AM	LPS File	717 KB
jl329.hkl	2020-05-11 12:19 AM	HKL File	2,681 KB
jl329.fab	2020-05-10 10:01 PM	FAB File	540 KB
jl329-mask.log	2020-05-10 10:01 PM	Text Document	5 KB
wgxJob.log	2020-05-10 9:18 PM	Text Document	1 KB
wgxTextServer.log	2020-05-10 9:17 PM	Text Document	1 KB
project.info	2020-05-10 9:17 PM	INFO File	7 KB
platon.input	2020-05-10 9:16 PM	INPUT File	2,722 KB
platon.fcf	2020-05-10 9:16 PM	FCF File	1,291 KB
jl329.pcf	2020-03-17 10:25 AM	PCF File	2 KB
mo_jl329.abs	2020-03-17 10:25 AM	ABS File	6 KB
mo_jl329_0m.ls	2020-03-17 10:24 AM	_LS File	72 KB

Annotations: A yellow arrow points from the text 'Text version of your validation response form' to the file 'jl329.chk'. Another yellow arrow points from the text 'Text version of your checkCIF report' to the file 'jl329.hkl'.

Text version of
your checkCIF
report



CheckCIF/Structure validation

Olex2 extension module CifPlus

Run checkCIF from PLATON



j1329C₃₉H₄₃ClF₃N₃Ni

a = 18.9031(13)
b = 26.3085(17)
c = 30.519(2)

α = 90°
 β = 90°
 γ = 90°

Z = 16
Z' = 2
V = 15177.2(18)

R₁ 6.72 %
wR₂ 24.18 %

d min (Mo) 0.70
Shift -0.446

I/ σ 22.5
Max Peak 4.4

Rint 4.52 %
Min Peak -0.5

complete 100 %
Goof 1.049

Warning: 5 atoms may be split and 0 atoms NPD

HomeWorkViewToolsInfo

SolveRefineDrawReport

Toolbox Work

CifPlus

ID = n/a

Love

Run Local CheckCif

0 | 10 | 2All

Sel Unique Labels

CIF j1329

Origination: Olex2 1.3
Collection ?
Reduction SAINT V8.40A (Bruker, 2019)

Device: Bruker APEX II area detector
Graphics: Olex2 1.3 (Dolomanov et al., 2009)
Solution SHELXT 2018/2 (Sheldrick, 2018)

CELL INFO OK
Publication Olex2 1.3 (Dolomanov et al., 2009)
Refinement: XL (Sheldrick, 2008)

μ = 0.626
Correction Details = SADABS-2016/2 (Bruker, 2016/2) was used for absorption correction. wR2(int) was 0.0556 before and 0.0470 after correction. The Ratio of minimum to maximum transmission is 0.9461. The W2 correction factor is Not present.

Peak = 4.364
Largest Shift = 0.446

Hole = -0.476
Mean Shift = 0.014

Restraints = 6
WGHT = 0.1 | 19.8

_refine_special_details = ?
_exptl_special_details = n/a

R1 = 0.0672
Shape prism
_av_R_equivalents = 0.0452
Total = 23172
MoK α (λ = 0.71073)

wR22 = 0.2418
Colour orange
_av_unetl/netl = 0.0444
I > 2 σ (I) = 16696
T = 90(2)

Data/Par = 18.31
0.41 x 0.38 x 0.21 mm³.
Use = 72.1 %
 Θ_{max} = 30.523
max/full = 0.999/1.000

SQUEEZE stuff failed!

All U_{eq} < 0.15
Run Checkcif now

All U_{eq} > 0.01

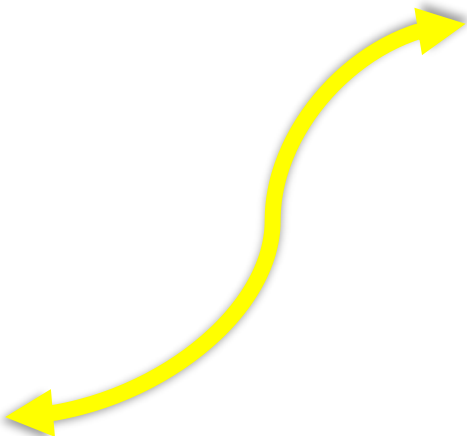
No _vrf_ RESPONSE in the cif file



CheckCIF/Structure validation

CifPlus

Click to edit directly into vrf!



i	Shape prism	Colour orange	0.41 x 0.38 x 0.21 mm ³ .
i	<u>_av_R_equivalents = 0.0452</u>		<u>_av_unetl/netl = 0.0444</u>
	Total = 23172	I > 2σ(I) = 16696	Use = 72.1%
	MoKα (λ = 0.71073)	T = 90(2)	Θ _{max} = 30.523 max/full = 0.999/1.000
i	SQUEEZE stuff failed!		
i	All U _{eq} < 0.15		All U _{eq} > 0.01
i	jl329: Rep: C39 H43 Cl F3 N3 Ni Calc: C39 H43 Cl F3 N3 Ni C-C = 0.0048		
	<u>080 ALERT 2 A Maximum Shift/Error 0.45 Why ?</u>		
	<u>094 ALERT 2 A Ratio of Maximum / Minimum Residual Density 9.17 Report</u>		
	<u>213 ALERT 2 A Atom F00P has ADP max/min Ratio 5.4 prolat</u>		
	<u>213 ALERT 2 A Atom C1 has ADP max/min Ratio 5.8 prolat</u>		
	<u>602 ALERT 2 A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info</u>		
	<u>971 ALERT 2 A Check Calcd Resid. Dens. 0.98A From</u>		
	<u>971 ALERT 2 A Check Calcd Resid. Dens. 0.98A From</u>		
	<u>971 ALERT 2 A Check Calcd Resid. Dens. 0.98A From</u>		
	<u>097 ALERT 2 B Large Reported Max. (Positive) Residual Density 4.36 eA-3</u>		
	<u>934 ALERT 3 B Number of (lobs- calc)/Sigma(W) > 10 Outliers .. 10 Check</u>		
	<u>971 ALERT 2 B Check Calcd Resid. Dens. 0.98A From</u>		
	<u>971 ALERT 2 B Check Calcd Resid. Dens. 0.98A From</u>		
	<u>213 ALERT 2 C Atom F1 has ADP max/min Ratio 3.8 prolat</u>		
	<u>213 ALERT 2 C Atom F00Q has ADP max/min Ratio 3.1 prolat</u>		
	<u>213 ALERT 2 C Atom F02J has ADP max/min Ratio 3.7 prolat</u>		
	<u>213 ALERT 2 C Atom F02H has ADP max/min Ratio 3.1 prolat</u>		
	<u>213 ALERT 2 C Atom F02I has ADP max/min Ratio 3.9 prolat</u>		
	<u>220 ALERT 2 C NonSolvent Resd 2 C Ueq(max) / Ueq(min) Range 3.9 Ratio</u>		
	<u>222 ALERT 3 C NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range 4.1 Ratio</u>		
	<u>234 ALERT 4 C Large Hirshfeld Difference C020... C1... 0.20 Ang</u>		



CheckCIF/Structure validation

Validation Response Forms

i	Shape prism	Colour orange	0.41 x 0.38 x 0.21 mm ³ .
i	<u>_av_R_equivalents</u> = 0.0452		<u>_av_unetl/netl</u> = 0.0444
	Total = 23172	I > 2σ(I) = 16696	Use = 72.1%
	MoKα (λ = 0.71073)	T = 90(2)	θ _{max} = 30.523 max/full = 0.999/1.000
i	SQUEEZE stuff failed!		
i	All U _{eq} < 0.15		All U _{eq} > 0.01
i	j1329: Rep: C39 H43 Cl F3 N3 Ni Calc: C39 H43 Cl F3 N3 Ni C-C = 0.0048		
	<u>080 ALERT 2 A Maximum Shift/Error 0.45 Why ?</u>		
	<u>094 ALERT 2 A Ratio of Maximum / Minimum Residual Density 9.17 Report</u>		
	<u>213 ALERT 2 A Atom F00P has ADP max/min Ratio 5.4 prolat</u>		
	<u>213 ALERT 2 A Atom C1 has ADP max/min Ratio 5.8 prolat</u>		
	<u>602 ALERT 2 A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info</u>		

Items to be entered into cif file

```
_olex2_diffraction_device 'Oxford Cryosystems'
_expt1_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_expt1_crystal_mounting_method 'The crystal was mounted on a mylar loop in oil'
_publ_contact_author_name            ''

_vrf_PLAT_602_j1329
;PROBLEM: VERY LARGE Solvent Accessible VOID[S] in Structure ! Info:
RESPONSE:
;
<
```

OK

Cancel



CheckCIF/Structure validation

Validation Response Forms

The ‘_’ in PLAT_620 is a syntax error! Horst is working on resolving this.

i	Shape prism	Colour orange	0.41 x 0.38 x 0.21 mm ³ .	
i	_av_R_equivalents = 0.0452		_av_unetl/netl = 0.0444	
	Total = 23172	I > 2σ(I) = 16696	Use = 72.1%	
	MoKα (λ = 0.71073)	T = 90(2)	Θ _{max} = 30.523	max/full = 0.999/1.000
i	SQUEEZE stuff failed!			
i	All U _{eq} < 0.15		All U _{eq} > 0.01	
i	jl329: Rep: C ₃₉ H ₄₃ Cl F ₃ N ₃ Ni Calc: C ₃₉ H ₄₃ Cl F ₃ N ₃ Ni C-C = 0.0048			
	<u>080 ALERT 2 A Maximum Shift/Error 0.45 Why ?</u>			
	<u>094 ALERT 2 A Ratio of Maximum / Minimum Residual Density 9.17 Report</u>			
	<u>213 ALERT 2 A Atom F00P has ADP max/min Ratio 5.4 prolat</u>			
	<u>213 ALERT 2 A Atom C1 has ADP max/min Ratio 5.8 prolat</u>			
	<u>602 ALERT 2 A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info</u>			

Items to be entered into cif file

```
_olex2_diffraction_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.



CifPlus

ID = n/a [Love](#)

Sel ☐ Unique ☒ Labels

CIF j329

Origination: Olex2 1.3 **Device:** Bruker APEX II area detector **CELL INFO OK**

Collection ? **Graphics:** Olex2 1.3 (Dolomanov et al., 2009) **Publication** Olex2 1.3 (Dolomanov et al., 2009)

Reduction SAINT V8.40A (Bruker, 2019) **Solution** SHELXT 2018/2 (Sheldrick, 2018) **Refinement:** XL (Sheldrick, 2008)

μ = 0.626 **μ_{mid} = 0.2** max = 0.7461 min = 0.7059 multi-scan

Correction Details = SADABS-2016/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0556 before and 0.0470 after correction. The Ratio of minimum to maximum transmission is 0.9461. The W2 correction factor is Not present.

Peak = 4.359 **Hole = -0.471** **Restraints = 6** 

Largest Shift = 0.107 **Mean Shift = 0.003** **WGHT = 0.1 | 20.5**

_refine_special_details = ?

_exptl_special_details = n/a

R1 = 0.0672 **wR22 = 0.2412** **Data/Par = 18.31** **GooF = 1.045**

Shape prism **Colour** orange **0.41 x 0.38 x 0.21 mm³.**

_av_R_equivalents = 0.0452 **_av_unetl/netl = 0.0444**

Total = 23172 **I > 2 σ (I) = 16696** **Use = 72.1%**

MoK α (λ = 0.71073) **T = 90(2)** **θ_{max} = 30.523** **max/full = 0.999/1.000**

SQUEEZE stuff failed!

All $U_{\text{eq}} < 0.15$ **All $U_{\text{eq}} > 0.01$**

[Run Checkcif now](#)

PROBLEM: VERY LARGE Solvent Accessible VOID[S] in Structure ! Info: RESPONSE: Blah blah blah

New CIF editor – FinalCif

<https://dkratzert.de/finalcif.html>

FC FinalCif v121

CIF File
[outside\Ihmels\hi005 - CCCW20\hi005-finalcif.cif] [Select File]

Recent Files

Search Key [Find a CIF keyword in the main table]

Equipment and Author Templates

APEX2 QUAZAR
Crystallographer Details
D8 VENTURE
Rigaku Spider

[New Template] [Edit Template] [Import]

[Import .cif, .pcf, .cif_od, .cfx or .sqf file]

Property Templates

Cell Measurement Temperature
Crystal Color
Crystal Cooling Device
Crystal Habit Description
Measurement Temperature
Molecular Graphics
Radiation Type
Sample environment
Twin relationship

[Edit Template] [New Template] [Import]

Data Name [hi005] [Append CIF] Space-Group Type [P2₁/n (14)] CCDC Number [] Sum Formula [C₂₅H₁₉N₅] [Help]

	CIF Value	From Data Source	Own Data
These below are already in:			
_refine_special_details			
_atom_sites_solution_hydrogens	geom		
_atom_sites_solution_primary	direct		
_audit_contact_author_address	Heiko Ihmels		
_audit_creation_date	2020-05-14		
_audit_creation_method	FinalCif V121 by Daniel Kratzert, Freiburg 2023, https://dkratzert.de/finalcif.html	FinalCif V121 by Daniel Kratzert, Freiburg 2023, https://dkratzert.de/finalcif.html	
_cell_angle_alpha	90		
_cell_angle_beta	99.232(2)		
_cell_angle_gamma	90		
_cell_formula_units_Z	4		
_cell_length_a	10.7046(8)		
_cell_length_b	15.0609(11)		
_cell_length_c	12.5922(10)		
_cell_measurement_reflns_used	8710		
_cell_measurement_temperature	90(2)		
_cell_measurement_theta_max	30.08		
_cell_measurement_theta_min	2.32		
_cell_volume	2003.8(3)		
_chemical_formula_moiety	C ₂₅ H ₁₉ N ₅ O ₅		
_chemical_formula_sum	C ₂₅ H ₁₉ N ₅ O ₅		
_chemical_formula_weight	413.41		
_computing_cell_refinement	SAINT v8.37A (Bruker, 2015)		
_computing_data_collection	Bruker BIS 2013.12.0.0/01-Nov-2013 && APEX2_2014.11-0		
_computing_data_reduction	SAINT v8.37A (Bruker, 2015)		
_computing_molecular_graphics	Olex2 1.3 (Dolomanov et al., 2009)		
_computing_publication_material	Olex2 1.3 (Dolomanov et al., 2009)		
_computing_structure_refinement	NoSpherA2		
_computing_structure_solution	SHELXT 2014/5 (Sheldrick, 2014)		
_diffraction_ambient_temperature	90(2)		

[Save CIF File] [Show Details] [CheckCIF] [Picture for Report] [COD Deposit] [Extract .hkl/.res File]

[Explore Directory] [Author Editor] [Edit Loops] [Make Report] [CCDC Deposit] [Options]



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EnCIFer enables users to validate CIFs and ensure their files are format-compliant for deposition with journals and databases or for storage in laboratory archives. EnCIFer should also be used to add information safely to CIFs without corrupting the strict syntax.

EnCIFer operates on single or multi-block CIFs allowing you to:

- Identify and correct syntax/format violations

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[CSD-Community](#)

Fields

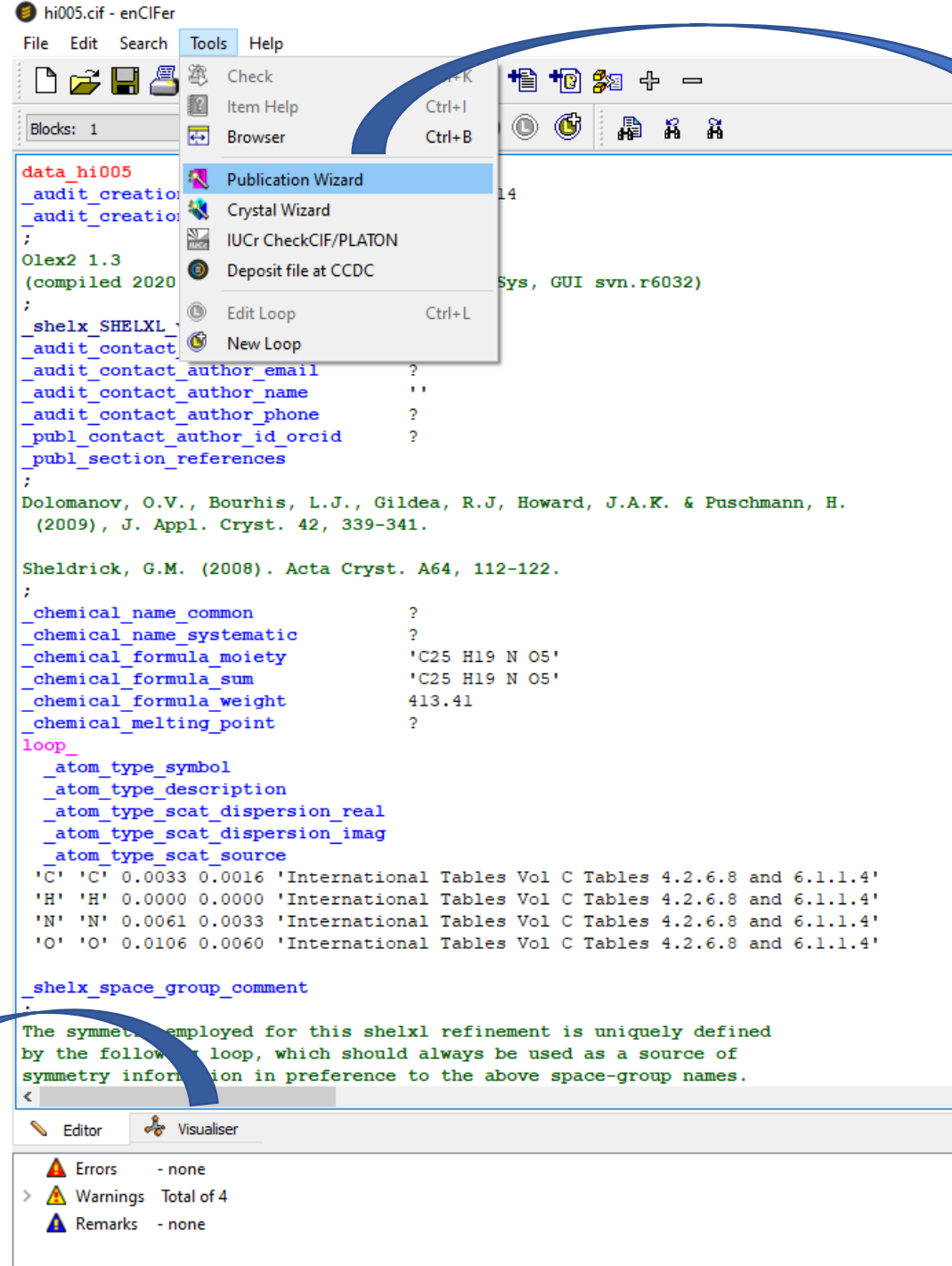
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Publication wizard to input pertinent information about authors, institutions, etc.

Same visualizer as found in Mercury!