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 1990		
I. D. Brown	The Crystallographic Information File (CIF) uses the self-defining STAR file structure.	become computer interpretable. This offers many possibilities for the automatic han-		
Brockhouse Institute for Materials	This requires the creation of a dictionary of data names and definitions. A basic dic-	dling of crystallographic information.		
Research, McMaster University, Hamilton, Ontario, Canada	tionary of terms needed to describe the crystal structures of small molecules was approved in 1991 and is currently used for	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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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.



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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), **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 <u>a new CIF will overwrite the previous CIF after each cycle</u>.











hi005.cif - Notepad Х File Edit Format View Help 'monoclinic' _space_group_crystal_system space group IT number 14 Information about the space group. space group name H-M alt 'P 1 21/n 1' '-P 2yn' _space_group_name_Hall 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' This (in addition to cell length a 10.7046(8)fractional coordinates) cell length b 15.0609(11)is all that's required to cell_length_c 12.5922(10) cell angle alpha 90 'build' the crystal. _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 A AA4



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_exptl_crystal_density_meas	?		
_exptl_crystal_density_method	?		
_exptl_crystal_description	?		
_exptl_crystal_F_000	864		
_exptl_crystal_size_max	0.2	Crystal stuff!	
_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_frac	tion_full 1.000		
_diffrn_reflns_Laue_measured_frac	tion_max 0.999		
_diffrn_reflns_limit_h_max	15		
_diffrn_reflns_limit_h_min	-15		
_diffrn_reflns_limit_k_max	18	Data stuff!	
_diffrn_reflns_limit_k_min	-21		
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What information is found in a CIF?

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Without files

What information is found in a CIF?

With files

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File Edit Format View Help		File Edit Format View Help			
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_exptl_crystal_F_000	864	expt1_crystal_cost iption	864		
_exptl_crystal_size_max	0.2		0.2		
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exptl crystal size min	0.09	_expti_crystal_size_min	0.15		
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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



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:

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.

a=10.7046(8) alpha=90	b=15.0609(11)	c=12.5922(10)		
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C25 H19 N O5	C25 H1	9 N 05		
413.41	413.41			
1.370	1.370			
4	4			
0.096	0.096			
864.0	864.0			
864.45				
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🔍 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 Adiffrn_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	1
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value	Please	Do	1
PLAT185 ALERT 1 A Missing cell_measurement_theta_max Value	Please	Do	1
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value	Please	Do	ł

Alert level C

PLAT052 ALERT 1 C	Info	on	Absorption	Correction	Method	Not	Given	Please Do	ļ
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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

- 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



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.

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 Adiffrn_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	1
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value	Please	Do	1
PLAT185 ALERT 1 A Missing cell measurement theta max Value	Please	Do	1
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value	Please	Do	1

Alert level C

PLAT052 ALERT 1 C Info on Absorption Correction Method Not Given Please Do ! IUCr) IUCr checkCIF procedure - Google Chrome _ \times ● journals.iucr.org/services/cif/checking/PLAT183.html se Do I IUCr II 5 Note **IUCr** Journals .3 Low 19 Info search IUCr Journals Q 0 home submit subscribe open access checkCIF procedure ight ed PLAT183 PLAT183 Type_1 Check for _cell_measured_refins_used value reported ta ent Please supply the value for _cell_measurement_reflns_used. E-alerts Twitter Facebook Follow IUCr Journals Search IUCr Journals Q doi All journals page Author volume Advanced search







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





Cut-and-paste the vrf into your CIF, edit in your own response at the '...', save and resubmit 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.



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Can access checkCIF from PLATON directly



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0	μ = 0.626	µ×mid = 0	.2 max =	0.7461 m	in = 0.7059	multi-scan
0	μ = 0.626 Correction De correction. wR to maximum train	µ×mid = 0 etails = SADA 2(int) was 0.0 nsmission is 0	.2 max = BS-2016/2 (Bru 556 before and .9461. The W2	0.7461 m uker,2016/2) v 10.0470 after correction fac	in = 0.7059 vas used for correction. T tor is Not pre	multi-scan absorption he Ratio of minimum sent.
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0	μ = 0.626 Correction Decorrection. wR3 to maximum train Peak = 4.364 Largest Shift	<pre>µ×mid = 0 atails = SADA 2(int) was 0.0 nsmission is 0 = 0.446</pre>	2 max = BS-2016/2 (Bru 556 before and 9461. The W2 Hole = -0.476 Mean Shift =	0.7461 m uker,2016/2) v 0.0470 after correction fac 0.014	in = 0.7059 vas used for correction. T tor is Not pre Restrain WGHT =	multi-scan absorption he Ratio of minimum issent. hts = 6
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	μ = 0.626 Correction De correction. wR2 to maximum trai Peak = 4.364 Largest Shift _refine_specia _exptl_specia R1 = 0.0672	<pre> µ×mid = 0 etails = SADA 2(int) was 0.0 nsmission is 0 = 0.446 al_details = 1 I_details = n/ wR22</pre>	2 max = BS-2016/2 (Bru 556 before and 9461. The W2 Hole = -0.476 Mean Shift = 2 a = 0.2418	0.7461 m uker,2016/2) v 0.0470 after correction fac 0.014 Data/Par =	in = 0.7059 vas used for correction. T tor is Not pre Restrain WGHT =	multi-scan absorption he Ratio of minimum issent. hts = 6 0.1 19.8 GooF = 1.049
	μ = 0.626 Correction De correction. wR to maximum train Peak = 4.364 Largest Shift _refine_specia _exptl_specia R1 = 0.0672 Shape prism	<pre>µ×mid = 0 etails = SADA 2(int) was 0.0 nsmission is 0 = 0.446 al_details = n/ wR22 Color</pre>	2 max = BS-2016/2 (Bru 556 before and 9461. The W2 Hole = -0.476 Mean Shift = 2 a = 0.2418 ur orange	0.7461 m Jker,2016/2) v 0.0470 after correction fac 0.014 Data/Par = 0.41 x 0.38	in = 0.7059 vas used for correction. T tor is Not pre Restrain WGHT = 18.31	multi-scan absorption he Ratio of minimum ssent. hts = 6 0.1 19.8 GooF = 1.049 3.
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	μ = 0.626 Correction De correction. wR to maximum train Peak = 4.364 Largest Shift _refine_specia _exptl_specia R1 = 0.0672 Shape prism _av_R_equiva Total = 23172	µ×mid = 0 etails = SADA 2(int) was 0.0 nsmission is 0 = 0.446 al_details = n/ wR22 Color lents = 0.045 I > 2(s	(sheidnick, 20 .2 max = BS-2016/2 (Bru 556 before and 9461. The W2 Hole = -0.476 Mean Shift = 7 a = 0.2418 ur orange 2 s(I) = 16696	0.7461 m uker,2016/2) v 0.0470 after correction fac 0.014 Data/Par = 0.41 x 0.38 _av_unet1	2000) iin = 0.7059 vas used for correction. T tor is Not pre- Restrain WGHT = 18.31 i x 0.21 mm^3 inetl = 0.044	multi-scan absorption he Ratio of minimum issent. its = 6 0.1 19.8 GooF = 1.049 3. 14 Use = 72.19
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	μ = 0.626 Correction De correction. wR to maximum trai Peak = 4.364 Largest Shift _refine_specia _exptl_specia R1 = 0.0672 Shape prism _av_R_equiva Total = 23172 MoK\a (λ = 0.7 SQUEEZE stuff All U _{eq} < 0.15	µ×mid = 0 tails = SADA 2(int) was 0.0 nsmission is 0 = 0.446 ial_details = n/ wR22 Colou lents = 0.045 I > 2\s 1073) T failed!	(sheddick, 20 .2 max = BS-2016/2 (Bru 556 before and .9461. The W2 Hole = -0.476 Mean Shift = ? a = 0.2418 ar orange 2 (i) = 16696 f = 90(2)	0.7461 m Jker,2016/2) v 0.0470 after correction fac 0.014 Data/Par = 0.41 x 0.38 _av_unetl 0 _{max} = 30 All U _{eo} > 0	2000) iin = 0.7059 vas used for correction. T tor is Not pre Restrain WGHT = 18.31 ix 0.21 mm^3 (netl = 0.044 .523 max .01	multi-scan absorption he Ratio of minimum issent. ints = 6 0.1 19.8 GooF = 1.049 3. 14 Use = 72.19 /full = 0.999/1.000
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CifPlus

Click to edit directly into vrf!

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0	Shape prism	Colour orange	0.41 x 0.38 x 0.21	I mm^3.
0	_av_R_equivalents	= 0.0452	_av_unetl/netl =	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
0	SQUEEZE stuff failed!			
0	All U _{eq} < 0.15		All U _{eq} > 0.01	
0	jl329: Rep: C39 H43 C	CI F3 N3 Ni Calc: C3	9 H43 CI F3 N3 Ni C	C-C = 0.0048
	080 ALERT 2 A Max	<u> kimum Shift/Error</u>	<u>0.45</u>	Why ?
	094 ALERT 2 A Rati	o of Maximum / Mi	<u>nimum Residual De</u>	ensity 9.17 Report
	213 ALERT 2 A Ato	m FOOP has ADP ma	ax/min Ratio 5.4	prolat_
	213 ALERT 2 A Ato	<u>m C1 has ADP max</u>	/min Ratio 5.8 pr	rolat_
	602 ALERT 2 A VER	Y LARGE Solvent A	ccessible VOID(S) i	in Structure ! Info
	971 ALERT 2 A Che	ck Calcd Resid. De	ns. 0.98A From	
	971 ALERT 2 A Che	ck Calcd Resid. De	ns. 0.98A From	
	971 ALERT 2 A Che	ck Calcd Resid. De	ns. 0.98A From	
	097 ALERT 2 B Larg	<u>e Reported Max. (</u>	<u>Positive) Residual [</u>	Density 4.36 eA-3
	934 ALERT 3 B Nun	hber of (lobs-lcalc)	/Sigma(W) > 10 Outl	iers 10 Check
	971 ALERT 2 B Che	ck Calcd Resid. De	<u>ns. 0.98A From</u>	
	971 ALERT 2 B Che	ck Calcd Resid. De	<u>ns. 0.98A From</u>	
	213 ALERT 2 C Ato	m F1 has ADP max/	min Ratio 3.8 pr	olat
	213 ALERT 2 C Ato	<u>m F00Q has ADP m</u>	ax/min Ratio 3.1	prolat
	213 ALERT 2 C Ato	m F02J has ADP ma	ax/min Ratio 3.7	prolat
	213 ALERT 2 C Ato	m F02H has ADP ma	ax/min Ratio 3.1	prolat_
	213 ALERT 2 C Ato	<u>m F02I has ADP ma</u>	x/min Ratio 3.9 j	orolat
	220 ALERT 2 C Non	Solvent Resd 2 C U	leq(max) / Ueq(min	<u>) Range 3.9 Ratio</u>
	222 ALERT 3 C Non	Solvent Resd 2 H U	iso(max)/Uiso(min)	Range 4.1 Ratio
	234 ALEDT A Clan	ne Hirehfeld Niffer	ance C020 C4 0.2	0 Ang

	6	Shape prism	Colour orange	0.41 x 0.38 x 0.2	1 mm^3.		
	6	av_R_equivalents	= 0.0452	_av_unetl/netl	= 0.0444		
		Total = 23172	I > 2\s(I) = 16696			Use = 72.1%	
		ΜοΚ\a (λ = 0.71073)	T = 90(2)	O _{max} = 30.523	max/full =	0.999/1.000	
	6	SQUEEZE stuff failed!					
	6) All U _{eq} < 0.15		All U _{eq} > 0.01			
	6) jl329: Rep: C39 H43 C	CI F3 N3 Ni Calc: C39	H43 CI F3 N3 Ni	C-C = 0.0048		
		080 ALERT 2 A Max	<u>kimum Shift/Error</u>	<u>0.4</u>	5 Why ?		
CheckCIF/Structure validation		094 ALERT 2 A Rati	<u>o of Maximum / Min</u>	<u>imum Residual D</u>	ensity 9.1	7 Report	
		213 ALERT 2 A Ato	m FOOP has ADP ma	<u>x/min Ratio 5.4</u>	prolat		
		213 ALERT 2 A Ato	m C1 has ADP max/r	<u>min Ratio 5.8 p</u>	<u>rolat</u>		
		602 ALERT 2 A VER	Y LARGE Solvent Ac	cessible VOID(S)	in Structure	<u>! Info</u>	
	Items to be entered into cif file			_			
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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
<pre>Alert level A THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less t Calculated sin(theta_max)/wavelength = 0.5378</pre>	chan 0.550
Alert level B PLAT415_ALERT_2_B Short Inter D-HH-X H47BH13B	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.