

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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

## Datablock: I

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Bond precision:    C-C = 0.0020 Å                      Wavelength=1.54187

Cell:                      a=8.8182(2)                      b=12.8387(3)                      c=14.1237(4)  
                                    alpha=82.167(6)                      beta=79.787(6)                      gamma=70.139(5)  
Temperature:    173 K

	Calculated	Reported
Volume	1475.06(8)	1475.06(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C23 H28 N3 O4, C7 H4 N O3 S, H2 O	C23 H28 N3 O4, C7 H4 N O3 S, H2 O
Sum formula	C30 H34 N4 O8 S	C30 H34 N4 O8 S
Mr	610.67	610.67
Dx, g cm <sup>-3</sup>	1.375	1.375
Z	2	2
Mu (mm <sup>-1</sup> )	1.466	1.466
F000	644.0	644.0
F000'	646.69	
h,k,lmax	10,15,17	10,15,16
Nref	5406	5291
Tmin,Tmax	0.619,0.864	0.455,0.864
Tmin'	0.425	

Correction method= # Reported T Limits: Tmin=0.455 Tmax=0.864  
AbsCorr = MULTI-SCAN

Data completeness= 0.979                      Theta(max)= 68.170

R(reflections)= 0.0337( 5009)                      wR2(reflections)= 0.0887( 5291)

S = 1.062                      Npar= 416

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

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### Alert level C

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full value Low	0.979	Why?
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	111 Report

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### Alert level G

PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	92%	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	4 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		16 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
2 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 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

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## checkCIF publication errors

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### Alert level A

PUBL004\_ALERT\_1\_A The contact author's name and address are missing,  
\_publ\_contact\_author\_name and \_publ\_contact\_author\_address.  
PUBL005\_ALERT\_1\_A \_publ\_contact\_author\_email, \_publ\_contact\_author\_fax and  
\_publ\_contact\_author\_phone are all missing.  
At least one of these should be present.  
PUBL006\_ALERT\_1\_A \_publ\_requested\_journal is missing  
e.g. 'Acta Crystallographica Section C'  
PUBL008\_ALERT\_1\_A \_publ\_section\_title is missing. Title of paper.  
PUBL009\_ALERT\_1\_A \_publ\_author\_name is missing. List of author(s) name(s).  
PUBL010\_ALERT\_1\_A \_publ\_author\_address is missing. Author(s) address(es).  
PUBL012\_ALERT\_1\_A \_publ\_section\_abstract is missing.  
Abstract of paper in English.

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### Alert level G

PUBL017\_ALERT\_1\_G The \_publ\_section\_references section is missing or  
empty.

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7 **ALERT level A** = Data missing that is essential or data in wrong format  
1 **ALERT level G** = General alerts. Data that may be required is missing

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## Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

## 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_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
```

PROBLEM: \_publ\_section\_abstract is missing.  
RESPONSE: ...  
;  
# end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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**PLATON version of 23/04/2018; check.def file version of 23/04/2018**

Datablock I - ellipsoid plot

