

# 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 = 0.0041 A	Wavelength=0.71073	
Cell:	a=5.7585(4)	b=16.7464(9)	c=14.1677(7)
	alpha=90	beta=100.300(5)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	1344.23(14)	1344.23(14)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C12 H10 Ag N O4 S2	C12 H10 Ag N O4 S2	
Sum formula	C12 H10 Ag N O4 S2	C12 H10 Ag N O4 S2	
Mr	404.20	404.20	
Dx,g cm-3	1.997	1.997	
Z	4	4	
Mu (mm-1)	1.820	1.820	
F000	800.0	800.0	
F000'	797.70		
h,k,lmax	7,21,18	7,21,18	
Nref	3095	3094	
Tmin,Tmax	0.728,0.834	0.809,1.000	
Tmin'	0.524		

Correction method= # Reported T Limits: Tmin=0.809 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.000

Theta(max)= 27.482

R(reflections)= 0.0293( 2652)

wR2(reflections)= 0.0653( 3094)

S = 1.070

Npar= 187

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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**

PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.74A From O1 -0.44 eA-3

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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 --S1 .	5.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Ag1 --S2_b .	17.0	s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Ag1 (I) .	1.11	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	1	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.2	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	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  
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
12 **ALERT level G** = General information/check it is not something unexpected

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

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## checkCIF publication errors

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**Alert level A**

PUBL012\_ALERT\_1\_A \_publ\_section\_abstract is missing.  
Abstract of paper in English.  
PUBL024\_ALERT\_1\_A The number of authors is greater than 9.  
Please specify the role of each of the co-authors  
for your paper.

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**Alert level G**

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

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2 **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_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PUBL024_GLOBAL
;
PROBLEM: The number of authors is greater than 9.
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 05/12/2020; check.def file version of 05/12/2020**

