

## checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: R28

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Bond precision:    C-C = 0.0036 A                      Wavelength=0.71070

Cell:                      a=10.9779(7)              b=5.7869(5)              c=12.1402(10)  
                                    alpha=90                      beta=92.349(4)              gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	770.60(10)	770.59(10)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C14 H19 N O5 S	C14 H19 N1 O5 S1
Sum formula	C14 H19 N O5 S	C14 H19 N O5 S
Mr	313.37	313.36
Dx,g cm-3	1.351	1.351
Z	2	2
Mu (mm-1)	0.230	0.230
F000	332.0	332.0
F000'	332.42	
h,k,lmax	13,7,15	13,7,15
Nref	3179[ 1752]	3156
Tmin,Tmax	0.962,0.982	0.916,0.966
Tmin'	0.921	

Correction method= MULTI-SCAN

Data completeness= 1.80/0.99                      Theta(max)= 26.441

R(reflections)= 0.0325( 2970)                      wR2(reflections)= 0.0695( 3156)

S = 1.014    Npar= Npar = 196

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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**

PLAT220\_ALERT\_2\_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.6 Ratio  
PLAT222\_ALERT\_3\_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 5.3 Ratio

● **Alert level G**

PLAT791\_ALERT\_4\_G The Model has Chirality at C1 ..... R Verify  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 2 Note

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  
2 **ALERT level G** = General information/check it is not something unexpected

0 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  
2 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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## Datablock: R35

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Bond precision: C-C = 0.0062 A Wavelength=0.71070  
Cell: a=5.7297(3) b=16.2240(9) c=17.5243(9)  
alpha=90 beta=90 gamma=90  
Temperature: 100 K

	Calculated	Reported
Volume	1629.04(15)	1629.04(15)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C14 H18 N4 O5 S	C14 H18 N4 O5 S1
Sum formula	C14 H18 N4 O5 S	C14 H18 N4 O5 S
Mr	354.39	354.38
Dx,g cm-3	1.445	1.445
Z	4	4
Mu (mm-1)	0.232	0.232
F000	744.0	744.0
F000'	744.85	
h,k,lmax	7,20,21	7,20,21
Nref	3362[ 1963]	3347
Tmin,Tmax	0.989,0.991	0.808,0.970
Tmin'	0.939	

Correction method= MULTI-SCAN

Data completeness= 1.71/1.00 Theta(max)= 26.462

R(reflections)= 0.0465( 2496)      wR2(reflections)= 0.1098( 3347)

S = 0.854

Npar= Npar = 223

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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.



**Alert level C**

PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0062 Ang.



**Alert level G**

PLAT791\_ALERT\_4\_G The Model has Chirality at C1 ..... R Verify

PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 4 Note

- 
- 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  
2 **ALERT level G** = General information/check it is not something unexpected

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



**Alert level A**

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.



**Alert level G**

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

empty.

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- 5 **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.

```
# start Validation Reply Form
_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 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.



