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: S

```
Bond precision:  C-C = 0.0049 A          Wavelength=0.71073

Cell:          a=9.1204(7)       b=10.8893(9)     c=11.1300(9)
               alpha=85.013(2)   beta=72.957(2)   gamma=67.152(2)
Temperature:   571 K
```

	Calculated	Reported
Volume	973.46(14)	973.46(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H17 Cl N5 S, S, H2 O	?
Sum formula	C18 H19 Cl N5 O S2	C18 H19 Cl N5 O S2
Mr	420.95	420.95
Dx,g cm-3	1.436	1.436
Z	2	2
Mu (mm-1)	0.430	0.430
F000	438.0	438.0
F000’	438.91	
h,k,lmax	10,12,13	10,12,13
Nref	3425	3387
Tmin,Tmax	0.835,0.980	
Tmin’	0.835	

```
Correction method= Not given

Data completeness= 0.989          Theta(max)= 24.994

R(reflections)= 0.0460( 2430)     wR2(reflections)= 0.1334( 3387)

S = 1.049                 Npar= 263
```

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 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 !

Alert level C

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !
PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.17 Do !
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00494 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X H1 .. H8AA .. 1.91 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N4A -- H5A ... Please Check

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Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT154_ALERT_1_G The s.u.’s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 3 Note

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5 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

7 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
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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_EXPT005_S
;
PROBLEM: _exptl_crystal_description is missing
RESPONSE: ...
;
_vrf_DIFF003_S
;
PROBLEM: _diffrn_measurement_device_type is missing
RESPONSE: ...
;
_vrf_PLAT183_S
;
PROBLEM: Missing _cell_measurement_reflns_used value ....     Please Do !
RESPONSE: ...
;
_vrf_PLAT184_S
;
PROBLEM: Missing _cell_measurement_theta_min value ......     Please Do !
RESPONSE: ...
;
_vrf_PLAT185_S
;
PROBLEM: Missing _cell_measurement_theta_max value ......     Please Do !
RESPONSE: ...
;
_vrf_PLAT052_S
```

```
;
PROBLEM: Info on Absorption Correction Method   Not Given     Please Do !
RESPONSE: ...
;
_vrf_PLAT057_S
;
PROBLEM: Correction for Absorption Required   RT(exp) ...       1.17 Do !
RESPONSE: ...
;
_vrf_PLAT340_S
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.00494 Ang.
RESPONSE: ...
;
_vrf_PLAT414_S
;
PROBLEM: Short Intra D-H..H-X       H1     ..  H8AA    ..       1.91 Ang.
RESPONSE: ...
;
_vrf_PLAT420_S
;
PROBLEM: D-H Without Acceptor       N4A    --  H5A    ...     Please Check
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 07/03/2016; check.def file version of 02/03/2016

Datablock S - ellipsoid plot