

## 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: BCd102\_1\_0m\_a

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Bond precision:    C-C = 0.0070 A

Wavelength=0.71073

Cell:                a=6.0444(4)                b=6.5440(5)                c=10.4117(5)  
                      alpha=106.940(4)        beta=95.623(4)        gamma=97.824(5)  
Temperature:        296 K

|                | Calculated       | Reported         |
|----------------|------------------|------------------|
| Volume         | 386.16(4)        | 386.15(4)        |
| Space group    | P -1             | P -1             |
| Hall group     | -P 1             | -P 1             |
| Moiety formula | C14 H12 Cd N4 S2 | C14 H12 Cd N4 S2 |
| Sum formula    | C14 H12 Cd N4 S2 | C14 H12 Cd N4 S2 |
| Mr             | 412.81           | 412.80           |
| Dx,g cm-3      | 1.775            | 1.775            |
| Z              | 1                | 1                |
| Mu (mm-1)      | 1.681            | 1.681            |
| F000           | 204.0            | 204.0            |
| F000'          | 203.48           |                  |
| h,k,lmax       | 7,7,12           | 7,7,12           |
| Nref           | 1308             | 1232             |
| Tmin,Tmax      | 0.817,0.845      |                  |
| Tmin'          | 0.817            |                  |

Correction method= Not given

Data completeness= 0.942

Theta(max)= 24.643

R(reflections)= 0.0345( 1148)

wR2(reflections)= 0.0772( 1232)

S = 1.017

Npar= 97

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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 B**

PLAT018\_ALERT\_1\_B \_diffn\_measured\_fraction\_theta\_max .NE. \_full ! Check

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**Alert level C**

THETM01\_ALERT\_3\_C The value of sine(theta\_max)/wavelength is less than 0.590  
Calculated sin(theta\_max)/wavelength = 0.5867  
PLAT052\_ALERT\_1\_C Info on Absorption Correction Method Not Given . Please Do !  
PLAT242\_ALERT\_2\_C Low Ueq as Compared to Neighbors for ..... C7 Check  
PLAT420\_ALERT\_2\_C D-H Without Acceptor N1 - H1B .. Please Check

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**Alert level G**

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 11 Report  
PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 2 Info  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 2 Report  
PLAT177\_ALERT\_4\_G The CIF-Embedded .res File Contains DELU Records 1 Report  
PLAT804\_ALERT\_5\_G Number of ARU-Code Packing Problem(s) in PLATON 1 Info  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 23 Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 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  
3 ALERT type 5 Informative message, check

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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*, 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.

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**PLATON version of 21/06/2015; check.def file version of 21/06/2015**

