

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Over0-8310-8134\_mk169

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: Over0-8310-8134\_mk169

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Bond precision:    C-C = 0.0047 A

Wavelength=0.71073

Cell:                a=8.5714(4)                b=10.4100(4)                c=11.9918(5)  
                      alpha=85.490(3)        beta=82.242(4)        gamma=76.835(4)  
Temperature:        100 K

	Calculated	Reported
Volume	1031.08(8)	1031.08(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C15 H14 N4 O, C6 H4 I2	C6 H4 I2, C15 H14 N4 O
Sum formula	C21 H18 I2 N4 O	C21 H18 I2 N4 O
Mr	596.19	596.19
Dx,g cm-3	1.920	1.920
Z	2	2
Mu (mm-1)	3.069	3.069
F000	572.0	572.0
F000'	570.28	
h,k,lmax	11,13,16	11,13,16
Nref	5198	5168
Tmin,Tmax	0.547,0.631	0.868,1.000
Tmin'	0.536	

Correction method= # Reported T Limits: Tmin=0.868 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.994

Theta(max)= 28.499

R(reflections)= 0.0332( 4144)

wR2(reflections)= 0.0570( 5168)

S = 1.062

Npar= 254

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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

PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min).

7 Note



### Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1 Report
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF .....	Please Check
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact I1S ..N1 .	3.23 Ang.
	x,y,z =	1_555 Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact I2S ..I2S	3.56 Ang.
	-1-x,2-y,-z =	2_475 Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	23 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1 Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	1 Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4 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
  - 9 **ALERT level G** = General information/check it is not something unexpected
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- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  - 4 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
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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* 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.

PLATON version of 19/10/2018; check.def file version of 15/10/2018

Datablock Over0-8310-8134\_mk169 - ellipsoid plot

