

# 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: MeDPP\_first\_merged\_a

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Bond precision:    C-C = 0.0068 A                      Wavelength=1

Cell:                      a=13.740(3)              b=6.850(2)              c=14.560(3)  
                            alpha=90              beta=94.56(3)              gamma=90

Temperature:              293 K

	Calculated	Reported
Volume	1366.0(6)	1366.0(6)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C16 H12 N2 O2 S2	?
Sum formula	C16 H12 N2 O2 S2	C64 H48 N8 O8 S8
Mr	328.40	1313.62
Dx,g cm-3	1.597	1.597
Z	4	1
Mu (mm-1)	1.024	0.000
F000	680.0	261.0
F000'	682.31	
h,k,lmax	21,10,22	21,10,22
Nref	5233	4493
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.859                      Theta(max)= 50.371

R(reflections)= 0.1913( 2988)              wR2(reflections)= 0.4895( 4493)

S = 1.637                      Npar= 201

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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 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.

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .	0.868	Why?
PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) .....	0.49	Report
PLAT183_ALERT_1_A Missing _cell_measurement_reflms_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 !
PLAT660_ALERT_1_A No Valid _diffrn_radiation_type Value Reported .		Please Do !
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value .....		Please Do !

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## Alert level B

PLAT082_ALERT_2_B High R1 Value .....	0.19	Report
PLAT230_ALERT_2_B Hirshfeld Test Diff for C1 --C00J .	8.5	s.u.

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## Alert level C

PLAT147_ALERT_1_C s.u. on Symmetry Constrained Cell Angle(s) .....		Please Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds .....	0.00679	Ang.

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## Alert level G

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...	4.00	Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	1.00000	Ang.
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =	3	Note
PLAT199_ALERT_1_G Reported _cell_measurement_temperature .....	293	Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature .....	293	Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C5	Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....	18	Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....	3.2	Low
PLAT981_ALERT_1_G No non-zero f" Anomalous Scattering Values Found		Please Check
PLAT986_ALERT_1_G No non-zero f' Anomalous Scattering Values Found		Please Check

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

- 14 **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  
4 **ALERT type 3** Indicator that the structure quality may be low  
4 **ALERT type 4** Improvement, methodology, query or suggestion  
0 **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.

