

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:      C-C = 0.0020 Å      Wavelength=0.71073

Cell:                      a=6.6838 (5)                      b=8.6592 (6)                      c=10.5128 (7)  
                              alpha=79.521 (2)                      beta=89.243 (2)                      gamma=86.626 (2)  
Temperature:              150 K

	Calculated	Reported
Volume	597.26 (7)	597.26 (7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C11 H8 Cl I N2 O2	C11 H8 Cl I N2 O2
Sum formula	C11 H8 Cl I N2 O2	C11 H8 Cl I N2 O2
Mr	362.54	362.54
Dx, g cm <sup>-3</sup>	2.016	2.016
Z	2	2
Mu (mm <sup>-1</sup> )	2.894	2.894
F000	348.0	348.0
F000'	347.47	
h, k, lmax	9, 12, 14	9, 12, 14
Nref	3375	3365
Tmin, Tmax	0.784, 0.944	0.648, 0.746
Tmin'	0.686	

Correction method= # Reported T Limits: Tmin=0.648 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.997      Theta(max)= 29.641

R(reflections)= 0.0174 ( 3189)	wR2(reflections)= 0.0411 ( 3365)
S = 1.034	Npar= 155

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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**

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.10	Report
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3	Report

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#### **Alert level G**

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT431_ALERT_2_G	Short Inter HL..A Contact I1 ..N1 .	3.35	Ang.
	x,-1+y,z =	1_545	Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	7	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	7	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  
2 **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  
4 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 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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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.

