

```
R(reflections)= 0.0410( 3441)      wR2(reflections)=
S = 1.082                        0.1102( 3654)
Npar= 176
```

---

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	3.90	Report
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N2	Check
PLAT245_ALERT_2_C	U(iso) H4B Smaller than U(eq) O4 by	0.011	Ang**2
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	43	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....	24	Note
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on Cul	1.45	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.81Ang From O4 .	0.43	eA-3

---



#### Alert level G

PLAT019_ALERT_1_G	_diffn_measured_fraction_theta_full/*_max < 1.0	0.993	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cul --O5 .	7.2	s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Cul (II) .	2.09	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	6	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2	Check

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
7 **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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
7 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

