

```
R(reflections)= 0.0343( 2331)      wR2(reflections)=
S = 1.117                        0.0794( 2611)
Npar= 136
```

---

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

PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	2.1	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.011	Ang.
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C1 - H1 .	1.12	Ang.
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C2 - H2 .	1.12	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1	Note
	C2 H9 B10 I3		
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	3.251	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	14	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.01Ang From I9	2.16	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.91Ang From C1 .	0.56	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.08Ang From C2 .	-0.55	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H1 .	-0.66	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H6 .	-0.56	eA-3

---



#### Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	12.31	Why ?
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C2	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1 - C2 .	1.64	Ang.
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	3	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	6	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.4	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

---

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
12 ALERT type 2 Indicator that the structure model may be wrong or deficient  
8 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

