

```
R(reflections)= 0.0519( 2660)      wR2(reflections)=
S = 1.142                        0.1355( 2925)
Npar= 235
```

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 B

THETM01_ALERT_3_B The value of $\sin(\theta_{\max})/\lambda$ is less than 0.575

Calculated $\sin(\theta_{\max})/\lambda = 0.5587$

Author Response: Old data from 2003.



Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low .	0.973	Why?
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.0133	Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	3.137	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.559	77	Report
PLAT977_ALERT_2_C Check Negative Difference Density on H11A .	-0.42	eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H11B .	-0.38	eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H11C .	-0.44	eA-3



Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	13.60	Why ?
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety	C11	Check
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still	83%	Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT930_ALERT_2_G FCF-based Twin Law [0 1 0] Est.d BASF	0.04	Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law [0 1 0] Est.d BASF	0.04	Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	4	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity	1.8	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
1 **ALERT level B** = A potentially serious problem, consider carefully
8 **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

- 1 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
8 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
-
-

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.

