

```
R(reflections)= 0.0938( 2330)      wR2(reflections)=
S = 1.061                        0.2847( 3168)
                                Npar= 202
```

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

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.154

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12	0.154	Report
PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of ...	2.500	Sigma
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.28	Report
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds	0.00667	Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # C15 H14 N2 O2 S3		1 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	7.813	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600		8 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .		1 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .	16.77	Check



Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.19	Report
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).		1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		5 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF		3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		2 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
10 **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
- 1 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
10 ALERT type 3 Indicator that the structure quality may be low
3 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.

