

```
R(reflections)= 0.0436( 2834)      wR2(reflections)=
S = 1.076                        0.1199( 3041)
Npar= 163
```

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

PLAT412_ALERT_2_C	Short Intra XH3 .. XHn	H9A	..H13A	.	1.82 Ang.	
			x,y,z =		1_555	Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd.	#			1	Note
	C13 H11 N3 O S					
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			2.240	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			10	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF			4	Note
PLAT977_ALERT_2_C	Check Negative Difference Density on H13A	.			-0.61	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H13B	.			-0.65	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H13C	.			-0.64	eA-3



Alert level G

PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical				?	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety			C13	Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				12	Info

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 4 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.

