

```
R(reflections)= 0.0246( 5174)      wR2(reflections)=
S = 1.074                        0.0578( 5530)
Npar= 307
```

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 A

PLAT431_ALERT_2_A Short Inter HL..A Contact I4 ..02 . 2.99 Ang.
3/2-x,-1/2+y,1/2-z = 2_645 Check

Alert level B

PLAT230_ALERT_2_B Hirshfeld Test Diff for N1 --C9 . 17.2 s.u.

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	5.5 Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1 H	Uiso(max)/Uiso(min) Range	5.5 Ratio
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	N1 Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	N4 Check
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond	C6 - C7	1.53 Ang.
PLAT911_ALERT_3_C	Missing FCF	Refl Between Thmin & STh/L=	0.600	17 Report
PLAT971_ALERT_2_C	Check Calcd	Resid. Dens.	0.75Ang From I2	1.81 eA-3

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij	Restrained non-H Atoms ...	3 Report
PLAT083_ALERT_2_G	SHELXL	Second Parameter in WGHT Unusually Large	11.13 Why ?
PLAT178_ALERT_4_G	The CIF-Embedded .res File	Contains SIMU Records	1 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File	Contains ISOR Records	1 Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Zn06 --06 .	12.7 s.u.
PLAT431_ALERT_2_G	Short Inter HL..A Contact	I1 ..01 .	3.18 Ang.
		1/2-x,1/2+y,1/2-z =	2_555 Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact	I2 ..05 .	3.13 Ang.
		1/2-x,1/2+y,1/2-z =	2_555 Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact	I3 ..05 .	3.08 Ang.
		1/2+x,1/2-y,-1/2+z =	4_665 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn06	(II) .	2.05 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	18 Note
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
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	3 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	.	9 Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation	has not Converged	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	.	2 Info

1 **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

17 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
3 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.

