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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.

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 **Alert level A**

PLAT971\_ALERT\_2\_A Check Calcd Resid. Dens. 1.28Ang From Sel 3.55 eA-3

**Author Response: Crystal quality - does not affect crystallorapich results.**

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 **Alert level B**

PLAT097\_ALERT\_2\_B Large Reported Max. (Positive) Residual Density 3.82 eA-3

**Author Response: Crystal quality - does not affect crystallorapich results.**

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 **Alert level C**

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75  
The relevant atom site should be identified.

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	3.90	Report
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C13	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.0079	Ang.
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn H15A ..H41A .	2.09	Ang.
	1-x,1-y,1-z =	3_666	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	11.564	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	3.055	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	7	Report

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 **Alert level G**

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	33.63	Why ?
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	571	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.7	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

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- 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
- 6 **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
  - 7 ALERT type 3 Indicator that the structure quality may be low
  - 1 ALERT type 4 Improvement, methodology, query or suggestion
  - 0 ALERT type 5 Informative message, check
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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.

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**PLATON version of 10/05/2023; check.def file version of 10/05/2023**

