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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 B

RINTA01\_ALERT\_3\_B The value of Rint is greater than 0.18  
Rint given 0.248  
PLAT020\_ALERT\_3\_B The Value of Rint is Greater Than 0.12 ..... 0.248 Report  
PLAT026\_ALERT\_3\_B Ratio Observed / Unique Reflections (too) Low .. 31% Check

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#### Alert level C

PLAT084\_ALERT\_3\_C High wR2 Value (i.e. > 0.25) ..... 0.33 Report  
PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00465 Ang.  
PLAT369\_ALERT\_2\_C Long C(sp2)-C(sp2) Bond C006 - C008 . 1.54 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 102.047 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.375 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 14.048 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.168 Check

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#### Alert level G

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G ALERT: check formula stoichiometry or atom site occupancies.  
From the CIF: \_cell\_formula\_units\_Z 9  
From the CIF: \_chemical\_formula\_sum C10.22 H10.22 F0.89 N0.44 O0.44  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	91.98	92.00	-0.02
H	91.98	92.00	-0.02
F	8.01	8.00	0.01
N	3.96	4.00	-0.04
O	3.96	4.00	-0.04

PLAT042\_ALERT\_1\_G Calc. and Reported Moiety Formula Strings Differ Please Check  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.4444 Check  
PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.13 Report  
PLAT333\_ALERT\_2\_G Large Aver C6-Ring C-C Dist C005 -C008 . 1.42 Ang.  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 50 Note  
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= 0.600 943 Note  
PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 1 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info

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

4 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  
10 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

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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 18/12/2021; check.def file version of 18/12/2021**

