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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 C**

PLAT413\_ALERT\_2\_C Short Inter XH3 .. XHn H13 ..H19B . 2.14 Ang.  
x,y,-1+z = 1\_554 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report

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● **Alert level G**

PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 1 Report  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.500 Check  
PLAT187\_ALERT\_4\_G The CIF-Embedded .res File Contains RIGU Records 1 Report  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of O13 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of C39 Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H13A Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H39A Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H39B Constrained at 0.5 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of H39C Constrained at 0.5 Check  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% Note  
PLAT398\_ALERT\_2\_G Deviating C-O-C Angle From 120 for O3 . 109.2 Degree  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O2 ..C17 . 2.91 Ang.  
-1/2+x,1/2-y,-z = 4\_455 Check  
PLAT789\_ALERT\_4\_G Atoms with Negative \_atom\_site\_disorder\_group # 6 Check  
PLAT822\_ALERT\_4\_G CIF-embedded .res Contains Negative PART Numbers 1 Check  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 5 Note  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 16 Note  
PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 1 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 22 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
4 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
11 ALERT type 4 Improvement, methodology, query or suggestion  
1 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 06/07/2023; check.def file version of 30/06/2023**

