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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

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12  
Rint given 0.132

PLAT020\_ALERT\_3\_C The Value of Rint is Greater Than 0.12 ..... 0.132 Report

PLAT085\_ALERT\_2\_C SHELXL Default Weighting Scheme is not Optimized Please Check

PLAT220\_ALERT\_2\_C NonSolvent Resd 2 C Ueq(max)/Ueq(min) Range 3.6 Ratio

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C02S Check

PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0042 Ang.

PLAT410\_ALERT\_2\_C Short Intra H...H Contact H14 ..H22 . 1.99 Ang.  
x,y,z = 1\_555 Check

PLAT410\_ALERT\_2\_C Short Intra H...H Contact H18 ..H46 . 1.99 Ang.  
x,y,z = 1\_555 Check

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### Alert level G

PLAT012\_ALERT\_1\_G N.O.K. \_shelx\_res\_checksum Found in CIF ..... Please Check

PLAT042\_ALERT\_1\_G Calc. and Reported Moiety Formula Strings Differ Please Check

PLAT244\_ALERT\_4\_G Low 'Solvent' Ueq as Compared to Neighbors of P001 Check

PLAT244\_ALERT\_4\_G Low 'Solvent' Ueq as Compared to Neighbors of P002 Check

PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 100 Note

PLAT790\_ALERT\_4\_G Centre of Gravity not Within Unit Cell: Resd. # 4 Note  
F6 P

PLAT802\_ALERT\_4\_G CIF Input Record(s) with more than 80 Characters 1 Info

PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !

PLAT965\_ALERT\_2\_G The SHELXL WEIGHT Optimisation has not Converged Please Check

PLAT967\_ALERT\_5\_G Note: Two-Theta Cutoff Value in Embedded .res .. 55.0 Degree

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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
- 8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 10 **ALERT level G** = General information/check it is not something unexpected
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- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 6 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
- 5 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.

