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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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.51	Report
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.01225	Ang.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N2 --H2B .		Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N3 --H3 .		Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	3.149	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	10	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	8	Report

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#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	25	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	22	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
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
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H3 ..N14 .	2.64	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H4 ..N12 .	2.63	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	10	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III) .	3.05	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	157	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	13	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law ( 1 0 0) Est.d BASF	0.47	Check
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	40	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	1.6	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check

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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  
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
19 **ALERT level G** = General information/check it is not something unexpected

- 0 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  
9 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

