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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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT214_ALERT_2_C	Atom C15 (Anion/Solvent) ADP max/min Ratio	4.6 prolat
PLAT223_ALERT_4_C	Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range	10.0 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C1 --C2	5.7 s.u.
PLAT245_ALERT_2_C	U(iso) H15 Smaller than U(eq) C15 by	0.037 Ang**2
PLAT350_ALERT_3_C	Short C-H (X0.96,N1.08A) C15 - H15	0.79 Ang.
PLAT350_ALERT_3_C	Short C-H (X0.96,N1.08A) C16 - H16	0.82 Ang.
PLAT350_ALERT_3_C	Short C-H (X0.96,N1.08A) C17 - H17	0.84 Ang.
PLAT350_ALERT_3_C	Short C-H (X0.96,N1.08A) C18 - H18	0.82 Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact H14 ..H15	1.91 Ang.
	x,y,z =	1_555 Check
PLAT410_ALERT_2_C	Short Intra H...H Contact H16 ..H17	1.93 Ang.
	x,y,z =	1_555 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600 150 Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H8A	-0.32 eA-3

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### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8 Report
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	8 Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1 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
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200 Report
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	71 Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	82% Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600 41 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	29 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.9 Low
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

0 **ALERT level B** = A potentially serious problem, consider carefully

13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

15 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

10 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

7 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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**Validation response form**

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT042_1Dy_auto
;
PROBLEM: Calc. and Reported MoietyFormula Strings Differ      Please Check
RESPONSE: ...
;
_vrf_PLAT214_1Dy_auto
;
PROBLEM: Atom C15          (Anion/Solvent) ADP max/min Ratio      4.6 prolat
RESPONSE: ...
;
_vrf_PLAT223_1Dy_auto
;
PROBLEM: Solv./Anion  Resd 2  H    Ueq(max)/Ueq(min) Range      10.0 Ratio
RESPONSE: ...
;
_vrf_PLAT230_1Dy_auto
;
PROBLEM: Hirshfeld Test Diff for    C1          --C2          .      5.7 s.u.
RESPONSE: ...
;
_vrf_PLAT245_1Dy_auto
;
PROBLEM: U(iso) H15          Smaller than U(eq) C15          by      0.037 Ang**2
RESPONSE: ...
;
_vrf_PLAT350_1Dy_auto
;
PROBLEM: Short  C-H (X0.96,N1.08A)  C15          -  H15          .      0.79 Ang.
RESPONSE: ...
;
_vrf_PLAT410_1Dy_auto
;
PROBLEM: Short Intra H...H Contact  H14          ..H15          .      1.91 Ang.
RESPONSE: ...
;
_vrf_PLAT911_1Dy_auto
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      150 Report
RESPONSE: ...
;
_vrf_PLAT977_1Dy_auto
;
PROBLEM: Check Negative Difference Density on H8A          .      -0.32 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

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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.

