



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.

---

**Alert level B**

PLAT111_ALERT_2_B	ADDSYM Detects New (Pseudo) Centre of Symmetry .	100	%Fit
PLAT112_ALERT_2_B	ADDSYM Detects New (Pseudo) Symm. Elem	d	100 %Fit
PLAT113_ALERT_2_B	ADDSYM Suggests Possible Pseudo/New Space Group	Fddd	Check

---

**Alert level C**

STRVA01\_ALERT\_4\_C                    Flack test results are ambiguous.  
From the CIF: `_refine_ls_abs_structure_Flack`      0.390  
From the CIF: `_refine_ls_abs_structure_Flack_su`      0.070

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18) .....	7.18	Note
PLAT234_ALERT_4_C	Large Hirshfeld Difference C2            --C3	0.16	Ang.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.01433	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=    0.600	2	Report
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	85	%

---

**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	16	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	11	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	15.60	Why ?
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5 )	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 2	2.91	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 3	2.09	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 4	3.44	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 5	2.56	Check
PLAT721_ALERT_1_G	Bond Calc      0.97000, Rep      0.96000 Dev...	0.01	Ang.
	C12A      -H12B            1.555    1.555 .....	#	69 Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cr1            (III)      .	2.82	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	122	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=    0.600	14	Note
PLAT916_ALERT_2_G	Hooft y and Flack x Parameter Values Differ by .	0.10	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	11	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

---

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 ALERT type 2 Indicator that the structure model may be wrong or deficient  
6 ALERT type 3 Indicator that the structure quality may be low  
14 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

---

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.

---

**PLATON version of 23/04/2018; check.def file version of 23/04/2018**

