



---

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 C**

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	4.3	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	4.1	Ratio
PLAT911_ALERT_3_C	Missing FCF	Refl	Between	Thmin & STh/L=	0.600	3	Report

---

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	13	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	9	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	15	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	13%	Note
PLAT791_ALERT_4_G	Model has Chirality at C5 (Sohnke SpGr)	R	Verify
PLAT791_ALERT_4_G	Model has Chirality at C12 (Sohnke SpGr)	S	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	111	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	1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	9	Info

---

0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
3 **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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
5 ALERT type 2 Indicator that the structure model may be wrong or deficient  
14 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

---

---

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 28/11/2022; check.def file version of 28/11/2022**

