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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**

PLAT213_ALERT_2_C	Atom C3	has ADP max/min Ratio	.....	3.1	prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	4.4	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1 H	Uiso(max)/Uiso(min) Range	4.7	Ratio
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C14	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C22	Check
PLAT911_ALERT_3_C	Missing FCF Refl	Between Thmin & STh/L=	0.600	11	Report

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● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle	Restraints on AtSite		4	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File	Contains DFIX Records		1	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File	Contains DANG Records		2	Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn1	(II)	.	2.29	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Mn2	(II)	.	2.09	Info
PLAT860_ALERT_3_G	Number of Least-Squares	Restraints	.....	3	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s)	Below Theta(Min).		3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections	Above STh/L=	0.600	38	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records	in Embedded .res File		1	Note
PLAT941_ALERT_3_G	Average HKL Measurement	Multiplicity	.....	3.3	Low
PLAT978_ALERT_2_G	Number C-C Bonds with	Positive Residual Density.		6	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  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
11 **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  
5 ALERT type 3 Indicator that the structure quality may be low  
3 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

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

