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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**

PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	Se1	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	Se4	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Nb2	Check
PLAT342_ALERT_3_C	Low	Bond Precision on C-C Bonds .....	0.0129	Ang.

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● **Alert level G**

PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	d	100	%Fit
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	d	100	%Fit
PLAT113_ALERT_2_G	ADDSYM Suggests Possible Pseudo/New Space Group		Fdd2	Check
	Check Model Parameter Symmetry for Reflection Data Support			
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		1.14	Ratio
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		60%	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		3.9	Low
PLAT963_ALERT_2_G	Both SHELXL WEIGHT Parameter Values Zero .....			Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		50.0	Degree
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  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
10 **ALERT level G** = General information/check it is not something unexpected

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
8 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
1 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 06/07/2023; check.def file version of 30/06/2023**

