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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

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio .....	8.44	Note
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	5.318	Check

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### Alert level G

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: H2 Na3 O9 P2 V1  
Atom count from \_chemical\_formula\_moiety: H4 Na6 O18 P4 V2

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for V1 (III) .	2.94	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	2	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	65%	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law ( 1 0 0) Est.d BASF	0.48	Check
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File 3 -9 3, 5 9 -3, -11 -7 5, -10 6 -6,	4	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	1.8	Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	50.0	Degree

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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  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
17 **ALERT level G** = General information/check it is not something unexpected

- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
2 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  
5 ALERT type 4 Improvement, methodology, query or suggestion  
4 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.



