
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

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.27	Report
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds	0.00864	Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance	2.524	Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	23	Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .	1	Check



Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	27.00	Why ?
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c	I2/c	Note
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...	3	Units
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File	10	Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	0	Info

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

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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT084_nia002_150k
;
PROBLEM: High wR2 Value (i.e. > 0.25) ..... 0.27 Report
RESPONSE: ...
;
_vrf_PLAT340_nia002_150k
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.00864 Ang.
RESPONSE: ...
;
_vrf_PLAT906_nia002_150k
;
PROBLEM: Large K Value in the Analysis of Variance ..... 2.524 Check
RESPONSE: ...
;
```

```

_vrf_PLAT911_nia002_150k
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      23 Report
RESPONSE: ...
;
_vrf_PLAT918_nia002_150k
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .      1 Check
RESPONSE: ...
;
# end Validation Reply Form

```

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 18/05/2022; check.def file version of 17/05/2022

