
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 A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.873 Why?

Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.588 1091 Report

Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590

Calculated sin(theta_max)/wavelength = 0.5879

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of 01 Check

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C59 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C57 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C60 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including 01 0.183 Check

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00479 Ang.

PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C57 - C58 . 1.35 Ang.

PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C58 - C59 . 1.42 Ang.

PLAT411_ALERT_2_C Short Inter H...H Contact H33 ..H57A . 2.00 Ang.

x,y,z = 1_555 Check

PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check

PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report

PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O1 . 107.4 Degree

PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info

PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info

PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 60% Note

PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 3 Note

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.5 Low

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

1 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

8 **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

9 ALERT type 3 Indicator that the structure quality may be low

7 ALERT type 4 Improvement, methodology, query or suggestion

0 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.

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_PLAT029_a_a
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .      0.873 Why?
RESPONSE: ...
;
# end Validation Reply Form
```

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

