
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 B

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections (too) Low .. 33% Check
PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01407 Ang.
PLAT411_ALERT_2_B Short Inter H...H Contact H14A ..H23 . 1.93 Ang.
5/2-x,-1/2+y,1/2-z = 2_745 Check



Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 0.798
PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.967 Why?
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT082_ALERT_2_C High R1 Value 0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.31 Report
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C27 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C28 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C25 -C30 . 1.37 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C13 - C14 . 1.35 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H13A ..H14B . 1.90 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_C Short Intra H...H Contact H13B ..H14A . 1.90 Ang.
x,y,z = 1_555 Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor N2 --H2A . Please Check
PLAT481_ALERT_4_C Long D...A H-Bond Reported C12 ..N6 . 3.78 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C29 H30 Cl F N6 O2



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT480_ALERT_4_G Long H...A H-Bond Reported H12A ..N6 . 3.08 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H27 ..O1 . 2.61 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints 1 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 22 Note

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

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

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

9 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

12 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
 6 ALERT type 4 Improvement, methodology, query or suggestion
 1 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_GOODF01_fcl
;
PROBLEM: The least squares goodness of fit parameter lies
RESPONSE: ...
;
_vrf_PLAT026_fcl
;
PROBLEM: Ratio Observed / Unique Reflections (too) Low ..          33% Check
RESPONSE: ...
;
_vrf_PLAT340_fcl
;
PROBLEM: Low Bond Precision on  C-C Bonds .....          0.01407 Ang.
RESPONSE: ...
;
_vrf_PLAT411_fcl
;
PROBLEM: Short Inter H...H Contact  H14A      ..H23      .          1.93 Ang.
RESPONSE: ...
;
_vrf_PLAT029_fcl
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .          0.967 Why?
RESPONSE: ...
;
_vrf_PLAT053_fcl
;
PROBLEM: Minimum Crystal Dimension Missing (or Error) ...          Please Check
RESPONSE: ...
;
_vrf_PLAT054_fcl
;
PROBLEM: Medium  Crystal Dimension Missing (or Error) ...          Please Check
RESPONSE: ...
;
_vrf_PLAT055_fcl
;
PROBLEM: Maximum Crystal Dimension Missing (or Error) ...          Please Check
RESPONSE: ...
;
_vrf_PLAT082_fcl
;
PROBLEM: High R1 Value .....          0.11 Report
RESPONSE: ...
;
```

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_vrf_PLAT084_fcl
;
PROBLEM: High wR2 Value (i.e. > 0.25) ..... 0.31 Report
RESPONSE: ...
;
_vrf_PLAT241_fcl
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of C27 Check
RESPONSE: ...
;
_vrf_PLAT242_fcl
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of C28 Check
RESPONSE: ...
;
_vrf_PLAT334_fcl
;
PROBLEM: Small <C-C> Benzene Dist. C25 -C30 . 1.37 Ang.
RESPONSE: ...
;
_vrf_PLAT360_fcl
;
PROBLEM: Short C(sp3)-C(sp3) Bond C13 - C14 . 1.35 Ang.
RESPONSE: ...
;
_vrf_PLAT410_fcl
;
PROBLEM: Short Intra H...H Contact H13A ..H14B . 1.90 Ang.
RESPONSE: ...
;
_vrf_PLAT420_fcl
;
PROBLEM: D-H Bond Without Acceptor N2 --H2A . Please Check
RESPONSE: ...
;
_vrf_PLAT481_fcl
;
PROBLEM: Long D...A H-Bond Reported C12 ..N6 . 3.78 Ang.
RESPONSE: ...
;
_vrf_PLAT790_fcl
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd. # 1 Note
RESPONSE: ...
;
# end Validation Reply Form

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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.

