
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

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C21 H21 Br P, Br
Rep.: Br, C21 H21 Br P
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report
3 0 0, 1 2 1, 2 0 2, -1 2 3, -2 0 4,



Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 5 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 3 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for Br2B --C1 . 6.2 s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 4% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H2B ..H1BD . 2.11 Ang.
x,y,z = 1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Br2B ..C14 . 3.32 Ang.
x,1+y,z = 1_565 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 4 Note
H1AA H1AB H1BC H1BD
PLAT860_ALERT_3_G Number of Least-Squares Restraints 30 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
1 0 0, 0 1 1, 0 0 2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 8 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 3 Note
3 0 0, 2 0 2, -2 0 4,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
0 0 2, 1 2 1,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.41 Note
Predicted wR2: Based on SigI**2 3.13 or SHELX Weight 7.42
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

- 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
14 **ALERT level G** = General information/check it is not something unexpected
- 1 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
5 ALERT type 3 Indicator that the structure quality may be low
3 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.

