
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

PLAT110_ALERT_2_B ADDSYM Detects Potential Lattice Translation ... ? Check

Author Response: Careful analysis using Xprep did not confirm this

PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

**Author Response: The structure was refined against HKLF5 file after
integrating the data using two domains**

 Alert level C

PLAT213_ALERT_2_C Atom C4	has ADP max/min Ratio	3.5 oblate
PLAT213_ALERT_2_C Atom C6	has ADP max/min Ratio	3.1 prolat
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor		2.1 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds		0.0178 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600		3 Report
PLAT914_ALERT_3_C No Bijvoet Pairs in FCF for Non-centro Structure		Please Check
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .		1 Check

 Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...		20 Report
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem C		100 %Fit

Author Response: Careful analysis using Xprep did not confirm this

PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group Cc Check
Note: (Pseudo) Lattice Translation Implemented

Author Response: Careful analysis using Xprep did not confirm this

PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records		4 Report
PLAT860_ALERT_3_G Number of Least-Squares Restraints		122 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 !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).		1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		12 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF		2 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File		3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		1.0 Low

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

2 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
12 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
3 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.

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