
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

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 7.2 Ratio

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_B Large Hirshfeld Difference C29 --C30 . 0.27 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.



Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 3.1 Ratio

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.3 Ratio

PLAT234_ALERT_4_C Large Hirshfeld Difference N4 --C7 . 0.24 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_C Large Hirshfeld Difference N4 --C8 . 0.23 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_C Large Hirshfeld Difference N8 --C48 . 0.20 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_C Large Hirshfeld Difference C8 --C9 . 0.22 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_C Large Hirshfeld Difference C19 --C20 . 0.23 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT234_ALERT_4_C Large Hirshfeld Difference C48 --C49 . 0.17 Ang.

Author Response: All allyl groups are severely disordered at the accessed temperature.

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C44 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including P1 0.114 Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C1 -C6 . 1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C21 -C26 . 1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C31 -C36 . 1.37 Ang.
PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C41 -C46 . 1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00559 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 24.132 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.064 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.032 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 33 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 28 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 20 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 18 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 10 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 18 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C9 --C10 . 7.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C39 --C40 . 8.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for C49 --C50 . 6.5 s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 26% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H17 ..H18A . 2.07 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H27 ..H28D . 2.09 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H57 ..H58A . 2.09 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H57 ..H58D . 2.03 Ang.
x,y,z = 1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 197 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 14 Note
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... 4 Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 54.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

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

19 ALERT type 2 Indicator that the structure model may be wrong or deficient
10 ALERT type 3 Indicator that the structure quality may be low
13 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

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

