
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

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check



Alert level C

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.2 Note
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00638 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.807 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 12 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.00A From O4 0.42 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.72A From O6 -0.45 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.85A From O1 -0.41 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H11 -0.32 eA-3



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 11 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 24.47 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 7 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 3 Report
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 24% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 10 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 94% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 10 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
8 **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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
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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_PLAT934_2

;

PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check

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RESPONSE: ...
;
_vrf_PLAT250_2
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.2 Note
RESPONSE: ...
;
_vrf_PLAT341_2
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.00638 Ang.
RESPONSE: ...
;
_vrf_PLAT906_2
;
PROBLEM: Large K Value in the Analysis of Variance .....      4.807 Check
RESPONSE: ...
;
_vrf_PLAT911_2
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.595      12 Report
RESPONSE: ...
;
_vrf_PLAT975_2
;
PROBLEM: Check Calcd Resid. Dens.  1.00A    From O4      0.42 eA-3
RESPONSE: ...
;
_vrf_PLAT976_2
;
PROBLEM: Check Calcd Resid. Dens.  0.72A    From O6      -0.45 eA-3
RESPONSE: ...
;
_vrf_PLAT977_2
;
PROBLEM: Check Negative Difference Density on H11      -0.32 eA-3
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.

