
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

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	5.286 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	18 Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	7 Note
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1 Check
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.92A From O6	-0.46 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	23.11 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	95% Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	11 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **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
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 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_PLAT341_1

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PROBLEM: Low Bond Precision on C-C Bonds 0.00638 Ang.

RESPONSE: ...

;

_vrf_PLAT906_1

;

PROBLEM: Large K Value in the Analysis of Variance 5.286 Check

RESPONSE: ...

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;
_vrf_PLAT911_1
;
PROBLEM: Missing FCF Refl Between Thmin & Sth/L=      0.595      18 Report
RESPONSE: ...
;
_vrf_PLAT913_1
;
PROBLEM: Missing # of Very Strong Reflections in FCF ....      7 Note
RESPONSE: ...
;
_vrf_PLAT934_1
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..      1 Check
RESPONSE: ...
;
_vrf_PLAT976_1
;
PROBLEM: Check Calcd Resid. Dens.  0.92A   From O6      -0.46 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.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock 1 - ellipsoid plot

