
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
PLAT112_ALERT_2_C	ADDSYM Detects New (Pseudo) Symm. Elem A	92 %Fit
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C40 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C42 Check
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn H17B ..H28 .	2.09 Ang.
	2-x,1-y,1-z =	3_766 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	12.829 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.474 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	6 Report



Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	9.34 Why ?
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O1 .	136.5 Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O2 .	137.5 Degree
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2 Note
	C2 H3 N	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3 Note
	C2 H3 N	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	4 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **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
3 ALERT type 3 Indicator that the structure quality may be low
5 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.

Datablock 1 - ellipsoid plot

