
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 A

PLAT355_ALERT_3_A Long O-H (X0.82,N0.98A) O6 - H6O . 1.15 Ang.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

STRVA01_ALERT_4_C Flack test results are ambiguous.

From the CIF: _refine_ls_abs_structure_Flack 0.400

From the CIF: _refine_ls_abs_structure_Flack_su 0.200

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.2 Note

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00471 Ang.

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & Sth/L= 0.600 66 Report

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 42 Note

Alert level G

PLAT019_ALERT_1_G _diffn_measured_fraction_theta_full/*_max < 1.0 0.997 Report

PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 0.80 mm

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check

PLAT303_ALERT_2_G Full Occupancy Atom H2O with # Connections 2.00 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 6 Note

PLAT791_ALERT_4_G Model has Chirality at C12 (Sohnke SpGr) S Verify

PLAT791_ALERT_4_G Model has Chirality at C15 (Sohnke SpGr) S Verify

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). 3 Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above Sth/L= 0.600 3 Note

PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note

PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 Info

1 **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

14 **ALERT level G** = General information/check it is not something unexpected

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

4 ALERT type 2 Indicator that the structure model may be wrong or deficient

5 ALERT type 3 Indicator that the structure quality may be low

6 ALERT type 4 Improvement, methodology, query or suggestion

1 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.

