
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

STRVA01_ALERT_4_C Flack parameter is too small
 From the CIF: _refine_ls_abs_structure_Flack -0.300
 From the CIF: _refine_ls_abs_structure_Flack_su 0.300
PLAT018_ALERT_1_C _diffn_measured_fraction_theta_max .NE. *_full ! Check
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 6.77 Note
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00596 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.596 18 Report



Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 9 Report
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 0.300 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0100 Report
PLAT189_ALERT_3_G A Non-default SAME Restraint Value for First Par 0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used 0.0100 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C11B Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12B Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13B Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14B Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11C Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12C Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13C Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14C Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10C Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11B Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12B Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14B Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14C Constrained at 0.65 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10D Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11C Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12C Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13C Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13D Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14D Constrained at 0.35 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H14E Constrained at 0.35 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 24% Note
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O3A . 107.3 Degree
PLAT480_ALERT_4_G Long H...A H-Bond Reported H17C ..02B . 2.64 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 5 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 133 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 59% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note

| | | | |
|-------------------|--|-----|------|
| PLAT933_ALERT_2_G | Number of HKL-OMIT Records in Embedded .res File | 3 | Note |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity | 3.4 | Low |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | 4 | Info |

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
43 **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
11 ALERT type 3 Indicator that the structure quality may be low
31 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.

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