
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

ABSMU01_ALERT_1_A The ratio of given/expected absorption coefficient lies
outside the range 0.90 <> 1.10
Calculated value of mu = 19.414
Value of mu given = 2.451

PLAT031_ALERT_4_A Refined Extinction Parameter Within Range 0.625 Sigma
PLAT051_ALERT_1_A Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 692.07 %
PLAT203_ALERT_2_A Negative Isotropic ADP for NA02 -0.001 Report
PLAT211_ALERT_2_A ADP of Atom Na02 is N.P.D. or (nearly) 2D . Please Check
PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.75A From Br01 3.54 eA-3
PLAT973_ALERT_2_A Check Calcd Positive Resid. Density on Na02 2.48 eA-3

Alert level B

PLAT021_ALERT_4_B Ratio Unique / Expected Reflections too High ... 1.087
PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.25 Note
PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pm-3m Check
Note: (Pseudo) Lattice Translation Implemented

PLAT927_ALERT_1_B Reported and Calculated wR2 Differ by -0.0066 Check

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT082_ALERT_2_C High R1 Value 0.11 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 3.05 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.44A From Na02 2.50 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.44A From Br01 2.27 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.25A From Br01 2.11 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 1.05A From Br01 -2.08 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 2.10A From Br01 -1.62 eA-3

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.19 Report
PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Translation ... ? Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem I 100 %Fit
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 1) 0.02 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 0.02 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 3 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check

7 **ALERT level A** = Most likely a serious problem - resolve or explain

4 **ALERT level B** = A potentially serious problem, consider carefully

8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 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
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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.

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_ABSMU01_aa20002x1_160721
;
PROBLEM: The ratio of given/expected absorption coefficient lies
RESPONSE: ...
;
_vrf_PLAT031_aa20002x1_160721
;
PROBLEM: Refined Extinction Parameter Within Range ..... 0.625 Sigma
RESPONSE: ...
;
_vrf_PLAT051_aa20002x1_160721
;
```

```
PROBLEM: Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      692.07 %
RESPONSE: ...
;
_vrf_PLAT203_aa20002x1_160721
;
PROBLEM: Negative Isotropic ADP for Na02      .....      -0.001 Report
RESPONSE: ...
;
_vrf_PLAT211_aa20002x1_160721
;
PROBLEM: ADP of Atom Na02      is N.P.D. or (nearly) 2D .      Please Check
RESPONSE: ...
;
_vrf_PLAT971_aa20002x1_160721
;
PROBLEM: Check Calcd Resid. Dens.  0.75A      From Br01      3.54 eA-3
RESPONSE: ...
;
_vrf_PLAT973_aa20002x1_160721
;
PROBLEM: Check Calcd Positive Resid. Density on      Na02      2.48 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

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

