
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 B



RINTA01_ALERT_3_B The value of Rint is greater than 0.18

Rint given 0.197

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 0.197 Report

PLAT149_ALERT_3_B s.u. on the beta Angle is Too Large 0.06 Degree

Alert level C

PLAT213_ALERT_2_C Atom C2 has ADP max/min Ratio 3.3 prolat

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C1 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C2 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N1 Check

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.7 Note

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.007 Ang.

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.985 Report

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info

PLAT013_ALERT_1_G N.O.K. _shelx_hkl_checksum Found in CIF Please Check

PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (II) 2.01 Info

PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 2 Info

PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 28 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
3 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

- 2 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
5 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
-

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_RINTA01_shelx
;
PROBLEM: The value of Rint is greater than 0.18
RESPONSE: ...
;
```

```

_vrf_PLAT020_shelx
;
PROBLEM: The Value of Rint is Greater Than 0.12 ..... 0.197 Report
RESPONSE: ...
;
_vrf_PLAT149_shelx
;
PROBLEM: s.u. on the beta Angle is Too Large ..... 0.06 Degree
RESPONSE: ...
;
_vrf_PLAT213_shelx
;
PROBLEM: Atom C2 has ADP max/min Ratio ..... 3.3 prolat
RESPONSE: ...
;
_vrf_PLAT220_shelx
;
PROBLEM: NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio
RESPONSE: ...
;
_vrf_PLAT241_shelx
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of C1 Check
RESPONSE: ...
;
_vrf_PLAT242_shelx
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of N1 Check
RESPONSE: ...
;
_vrf_PLAT250_shelx
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.7 Note
RESPONSE: ...
;
_vrf_PLAT341_shelx
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.007 Ang.
RESPONSE: ...
;
_vrf_PLAT905_shelx
;
PROBLEM: Negative K value in the Analysis of Variance ... -0.985 Report
RESPONSE: ...
;
# end Validation Reply Form

```

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.

