
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

PLAT242_ALERT_2_B	Low	'MainMol' Ueq as Compared to Neighbors of	C15	Check
PLAT601_ALERT_2_B	Unit Cell Contains Solvent Accessible VOIDS of .		103	Ang**3

Alert level C

PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please	Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please	Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please	Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		3.59	Report
PLAT213_ALERT_2_C	Atom O5	has ADP max/min Ratio	3.5	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	4.6	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H	Uiso(max)/Uiso(min) Range	5.4	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		06	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C10	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Cd1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C13	Check

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		6	Note
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please	Do !
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large		0.11	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cd1 --O3 .		8.1	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cd1 --O5_a .		50.5	s.u.
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C14	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C16	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd1 (II) .		2.02	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		4	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL-		2019/2	Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 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
3 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
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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_PLAT242_1
;
PROBLEM: Low      'MainMol' Ueq as Compared to Neighbors of      C15 Check
RESPONSE: ...
;
_vrf_PLAT601_1
;
PROBLEM: Unit Cell Contains Solvent Accessible VOIDS of .      103 Ang**3
RESPONSE: ...
;
_vrf_PLAT053_1
;
PROBLEM: Minimum Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT054_1
;
PROBLEM: Medium   Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT055_1
;
PROBLEM: Maximum Crystal Dimension Missing (or Error) ...      Please Check
RESPONSE: ...
;
_vrf_PLAT094_1
;
PROBLEM: Ratio of Maximum / Minimum Residual Density ....      3.59 Report
RESPONSE: ...
;
_vrf_PLAT213_1
;
PROBLEM: Atom O5                has ADP max/min Ratio .....      3.5 prolat
RESPONSE: ...
;
_vrf_PLAT220_1
;
PROBLEM: NonSolvent   Resd 1   C   Ueq(max)/Ueq(min) Range      4.6 Ratio
RESPONSE: ...
;
_vrf_PLAT222_1
;
PROBLEM: NonSolvent Resd 1   H   Uiso(max)/Uiso(min) Range      5.4 Ratio
RESPONSE: ...
;
_vrf_PLAT241_1
;
PROBLEM: High      'MainMol' Ueq as Compared to Neighbors of      O6 Check
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.

