

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

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.0257 Ang.

Alert level C

RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25

Weighted R factor given 0.260

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low 0.963 Note

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.26 Why ?

PLAT234_ALERT_4_C Large Hirshfeld Difference C1 -- C2 .. 0.25 Ang.

PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for 02 Check

Author Response: This Alert is due to low quality data and higher values of thermal parameters.

PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C2 Check

Author Response: This Alert is due to low quality data and higher values of thermal parameters.

PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C12 Check

Author Response: This Alert is due to low quality data and higher values of thermal parameters.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for N1 Check

Author Response: This Alert is due to low quality data and higher values of thermal parameters.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C1 Check

Author Response: This Alert is due to low quality data and higher values of thermal parameters.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C8 Check

Author Response: This Alert is due to low quality data and higher values of thermal parameters.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C11 Check

Author Response: This Alert is due to low quality data and higher values of thermal parameters.

PLAT332_ALERT_2_C	Large Phenyl C-C Range	C1	-C6	0.17	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond	C14	- C14_c ...	1.42	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance		14.198	Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance		2.143	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.593		88	Why ?
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.12A	From C11	1.83	eA-3

Author Response: This Alert is due to presence of residual density in the presence of heavy metal atom (Ag).

PLAT971_ALERT_2_C	Check Calcd Residual Density	1.17A	From C12	1.68	eA-3
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Author Response: This Alert is due to presence of residual density in the presence of heavy metal atom (Ag).

PLAT971_ALERT_2_C	Check Calcd Residual Density	1.13A	From C3	1.67	eA-3
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Author Response: This Alert is due to presence of residual density in the presence of heavy metal atom (Ag).

PLAT971_ALERT_2_C	Check Calcd Residual Density	1.21A	From C9	1.63	eA-3
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Author Response: This Alert is due to presence of residual density in the presence of heavy metal atom (Ag).

PLAT971_ALERT_2_C	Check Calcd Residual Density	1.44A	From S1	1.52	eA-3
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Author Response: This Alert is due to presence of residual density in the presence of heavy metal atom (Ag).

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Dimension		2	Info
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF				Please Do !
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.			50.45	Why ?
PLAT153_ALERT_1_G	The su's on the Cell Axes are Equal		0.00500	Ang.
PLAT909_ALERT_3_G	Percentage of Observed Data at Theta(Max) still			57	%
PLAT910_ALERT_3_G	Missing # of FCF Reflections Below Th(Min)		4	Why ?

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 21 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 6 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 1 ALERT type 4 Improvement, methodology, query or suggestion
 2 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*, 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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