
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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.540 Why?

**Author Response: Multigrain sample in a diamond anvil cell (DAC).
Aperture is limited by the DAC geometry.**

 Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 176 Report

**Author Response: Multigrain sample in a diamond anvil cell (DAC).
Aperture is limited by the DAC geometry.**

PLAT975_ALERT_2_B Check Calcd Resid. Dens. 0.85Ang From N2 . 1.77 eA-3

**Author Response: Multigrain sample in a DAC. Strong electronic contrast
between Bi and N and limited completeness.**

PLAT975_ALERT_2_B Check Calcd Resid. Dens. 0.70Ang From N2 . 1.61 eA-3

**Author Response: Multigrain sample in a DAC. Strong electronic contrast
between Bi and N and limited completeness.**

PLAT976_ALERT_2_B Check Calcd Resid. Dens. 1.03Ang From N1 . -1.63 eA-3

**Author Response: Multigrain sample in a DAC. Strong electronic contrast
between Bi and N and limited completeness.**

 Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT051_ALERT_1_C	Mu(calc) and Mu(CIF) Ratio	Differs from 1.0 by .	1.24 %
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
PLAT127_ALERT_1_C	Implicit Hall Symbol	Inconsistent with Explicit -P	-2xab;- Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance	...	-0.205 Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF		7 Note
PLAT921_ALERT_1_C	R1 in the CIF and FCF	Differ by	0.0020 Check
PLAT926_ALERT_1_C	Reported and Calculated R1	Differ by	0.0020 Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.72Ang From Bi2	2.38 eA-3

PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.79Ang	From	Bi1	2.31	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.64Ang	From	Bi2	2.25	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.79Ang	From	Bi1	2.04	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.85Ang	From	N1	1.99	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.23Ang	From	N1	1.94	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.92Ang	From	N2	1.90	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.82Ang	From	Bi2	1.90	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.00Ang	From	N1	1.80	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.37Ang	From	N2	1.80	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.85Ang	From	N2	1.77	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.68Ang	From	Bi2	1.76	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.06Ang	From	Bi1	1.75	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.95Ang	From	N1	1.74	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.95Ang	From	N1	1.74	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.97Ang	From	N1	1.74	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.72Ang	From	N2	1.73	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.76Ang	From	N2	1.68	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.61Ang	From	Bi1	1.68	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.61Ang	From	Bi1	1.68	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.63Ang	From	N1	1.68	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.22Ang	From	Bi2	1.66	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.46Ang	From	N1	1.66	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.70Ang	From	N2	1.61	eA-3
PLAT971_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.35Ang	From	N1	1.61	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.61Ang	From	Bi2	-2.32	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.62Ang	From	Bi2	-2.32	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.29Ang	From	Bi2	-2.27	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.31Ang	From	N2	-2.09	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.07Ang	From	Bi1	-2.05	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.34Ang	From	N1	-2.03	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.18Ang	From	Bi1	-1.97	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.14Ang	From	Bi1	-1.97	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.05Ang	From	Bi1	-1.96	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.18Ang	From	Bi2	-1.90	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.18Ang	From	Bi2	-1.90	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.22Ang	From	N2	-1.88	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.18Ang	From	Bi1	-1.81	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.10Ang	From	Bi2	-1.80	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.96Ang	From	Bi2	-1.71	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.29Ang	From	Bi1	-1.70	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.27Ang	From	Bi2	-1.70	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.29Ang	From	Bi2	-1.68	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.42Ang	From	Bi1	-1.66	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	0.22Ang	From	Bi2	-1.66	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.24Ang	From	N1	-1.65	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.67Ang	From	N1	-1.64	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.16Ang	From	N1	-1.63	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.03Ang	From	N1	-1.63	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Resid.	Dens.	1.62Ang	From	Bi1	-1.61	eA-3
PLAT992_ALERT_5_C	Repd & Actual	_reflns_number_gt	Values Differ by					39	Check



Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !

PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.29090	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi1 (III) .	2.31	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Bi2 (III) .	2.26	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	452	Note
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	3	Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	8	Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ	3	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	8	Units
PLAT984_ALERT_1_G	The Bi-f' = -0.8723 Deviates from the B&C-Value	-0.8028	Check
PLAT985_ALERT_1_G	The Bi-f" = 2.4794 Deviates from the B&C-Value	2.4568	Check

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
 4 **ALERT level B** = A potentially serious problem, consider carefully
 61 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 18 **ALERT level G** = General information/check it is not something unexpected
- 17 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 53 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
 7 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.

Datablock 1 - ellipsoid plot

