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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.

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 **Alert level A**

PLAT029\_ALERT\_3\_A \_diffn\_measured\_fraction\_theta\_full value Low . 0.919 Why?

**Author Response: The data were collected on MX14-2 beamline (Bessy II, Berlin) and spindle axis rotation was the only available strategy resulting in slightly lowered completeness for triclinic and sometimes also monoclinic crystals.**

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 **Alert level B**

PLAT430\_ALERT\_2\_B Short Inter D...A Contact O18 ..O18 . 2.78 Ang.  
1-x,-y,-z = 2\_655 Check  
PLAT911\_ALERT\_3\_B Missing FCF Refl Between Thmin & STh/L= 0.600 473 Report

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 **Alert level C**

PLAT213\_ALERT\_2\_C Atom F10 has ADP max/min Ratio ..... 3.4 prolat  
PLAT213\_ALERT\_2\_C Atom F11 has ADP max/min Ratio ..... 3.2 prolat  
PLAT213\_ALERT\_2\_C Atom F12 has ADP max/min Ratio ..... 3.2 prolat

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 **Alert level G**

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 2 Report  
PLAT066\_ALERT\_1\_G Predicted and Reported Tmin&Tmax Range Identical ? Check  
PLAT092\_ALERT\_4\_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.79990 Ang.  
PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree  
PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 2 Report  
PLAT242\_ALERT\_2\_G Low 'MainMol' Ueq as Compared to Neighbors of C3A Check  
PLAT242\_ALERT\_2\_G Low 'MainMol' Ueq as Compared to Neighbors of C20A Check  
PLAT242\_ALERT\_2\_G Low 'MainMol' Ueq as Compared to Neighbors of C34A Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F7 Constrained at 0.7 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F8 Constrained at 0.7 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F9 Constrained at 0.7 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F10 Constrained at 0.3 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F11 Constrained at 0.3 Check  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of F12 Constrained at 0.3 Check  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1 ) 5% Note  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O22 ..C18 . 2.97 Ang.  
-x,-y,-z = 2\_555 Check  
PLAT432\_ALERT\_2\_G Short Inter X...Y Contact O22 ..C19 . 2.98 Ang.  
-x,-y,-z = 2\_555 Check  
PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact F1 ..F7 . 2.76 Ang.  
1-x,1-y,1-z = 2\_666 Check  
PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact F1 ..F12 . 2.80 Ang.

	1+x,1+y,z =	1_665	Check
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	12	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT898_ALERT_4_G	Second Reported H-M Symbol in CIF Ignored .....		! Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	183	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.4	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	7	Info
PLAT984_ALERT_1_G	The C-f' = 0.0033 Deviates from the B&C-Value	0.0043	Check
PLAT984_ALERT_1_G	The F-f' = 0.0186 Deviates from the B&C-Value	0.0225	Check
PLAT984_ALERT_1_G	The N-f' = 0.0063 Deviates from the B&C-Value	0.0082	Check
PLAT984_ALERT_1_G	The O-f' = 0.0113 Deviates from the B&C-Value	0.0142	Check

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 14 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  
 11 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.

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**PLATON version of 19/02/2022; check.def file version of 19/02/2022**

