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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 B

PLAT029\_ALERT\_3\_B \_diffn\_measured\_fraction\_theta\_full value Low . 0.956 Why?

**Author Response: Since the Pohang Accelerator Laboratory 2D Beamline goniostat has only one omega-axis, diffn\_measured\_fraction\_theta\_full is not fully covered as 0.956, especially for the low symmetry such as triclinic system. As this is an inherent problem, other command and option were not helpful to improve the completeness.**

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#### Alert level C

PLAT213\_ALERT\_2\_C Atom C5B has ADP max/min Ratio ..... 3.6 oblate  
PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including O3B 0.105 Check  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.214 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 275 Report  
PLAT977\_ALERT\_2\_C Check Negative Difference Density on H7A -0.34 eA-3

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#### Alert level G

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

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 30 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 15 Report  
PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 2 Info  
PLAT063\_ALERT\_4\_G Crystal Size Possibly too Large for Beam Size .. 0.86 mm  
PLAT092\_ALERT\_4\_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.63000 Ang.  
PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.03 Degree  
PLAT168\_ALERT\_4\_G The CIF-Embedded .res File Contains EXYZ Records 3 Report  
PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 3 Report  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 18 Report  
PLAT173\_ALERT\_4\_G The CIF-Embedded .res File Contains DANG Records 18 Report  
PLAT174\_ALERT\_4\_G The CIF-Embedded .res File Contains FLAT Records 6 Report  
PLAT177\_ALERT\_4\_G The CIF-Embedded .res File Contains DELU Records 3 Report  
PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 3 Report  
PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 2 Report  
PLAT187\_ALERT\_4\_G The CIF-Embedded .res File Contains RIGU Records 6 Report  
PLAT300\_ALERT\_4\_G Atom Site Occupancy of Zn2 Constrained at 0.5 Check  
PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1 ) 20% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 3 ) 100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 4 ) 100% Note  
PLAT413\_ALERT\_2\_G Short Inter XH3 .. XHn H25B ..H2B3 . 2.10 Ang.  
1-x,1-y,1-z = 2\_666 Check  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 36 Note  
PLAT779\_ALERT\_4\_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 17.26 Deg.  
ZN2 -N1 -ZN2 1\_555 1\_555 2\_766 ..... # 43 Check  
PLAT779\_ALERT\_4\_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 17.57 Deg.

|                   |                                                  |      |       |       |       |       |   |        |       |
|-------------------|--------------------------------------------------|------|-------|-------|-------|-------|---|--------|-------|
| ZN2               | -N2                                              | -ZN2 | 1_555 | 1_555 | 2_766 | ..... | # | 49     | Check |
| PLAT804_ALERT_5_G | Number of ARU-Code Packing Problem(s) in PLATON  |      |       |       |       |       |   | 1      | Info  |
| PLAT811_ALERT_5_G | No ADDSYM Analysis: Too Many Excluded Atoms .... |      |       |       |       |       |   | !      | Info  |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints .....         |      |       |       |       |       |   | 312    | Note  |
| 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  |      |       |       |       |       |   | 354    | Note  |
| PLAT941_ALERT_3_G | Average HKL Measurement Multiplicity .....       |      |       |       |       |       |   | 2.0    | Low   |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. |      |       |       |       |       |   | 6      | Info  |
| PLAT984_ALERT_1_G | The Zn-f' = 0.3273 Deviates from the B&C-Value   |      |       |       |       |       |   | 0.3261 | Check |
| PLAT985_ALERT_1_G | The Zn-f" = 1.1646 Deviates from the B&C-Value   |      |       |       |       |       |   | 1.1614 | Check |

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
8 ALERT type 2 Indicator that the structure model may be wrong or deficient  
6 ALERT type 3 Indicator that the structure quality may be low  
19 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock P-1\_a - ellipsoid plot

