

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) RX

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: RX

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Bond precision:      C-C = 0.0114 Å      Wavelength=0.71073

Cell:                      a=9.5365(4)                      b=10.4289(3)                      c=18.2694(7)  
                              alpha=96.932(1)                      beta=90.811(2)                      gamma=108.331(1)  
Temperature:              200 K

	Calculated	Reported
Volume	1709.56(11)	1709.56(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C14 H19 N3 O4), 5(H2 O)	2(C14 H19 N3 O4), 5(H2 O)
Sum formula	C28 H48 N6 O13	C28 H48 N6 O13
Mr	676.72	676.72
Dx, g cm <sup>-3</sup>	1.315	1.315
Z	2	2
Mu (mm <sup>-1</sup> )	0.104	0.104
F000	724.0	724.0
F000'	724.40	
h, k, lmax	9, 10, 18	8, 10, 16
Nref	3632	1361
Tmin, Tmax	0.985, 0.998	0.875, 0.945
Tmin'	0.985	

Correction method= # Reported T Limits: Tmin=0.875 Tmax=0.945  
AbsCorr = MULTI-SCAN

Data completeness= 0.375      Theta(max)= 20.911

R(reflections)= 0.0353( 1206)	wR2(reflections)= 0.0847( 1361)
S = 1.049	Npar= 420

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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**

THETM01\_ALERT\_3\_A The value of  $\sin(\theta_{\max})/\lambda$  is less than 0.550  
Calculated  $\sin(\theta_{\max})/\lambda = 0.5022$

**Author Response: Due to the very low diffraction properties of the crystal, which was the only one (out of >10 attempts) that we could find in the batch.**

PLAT029\_ALERT\_3\_A  $\text{\_diffraction\_measured\_fraction\_theta\_full}$  value Low . 0.375 Why?

**Author Response: This is likely related to the weak diffraction of the crystal.**

PLAT088\_ALERT\_3\_A Poor Data / Parameter Ratio ..... 3.24 Note

**Author Response: This is likely related to the weak diffraction of the crystal.**

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#### **Alert level B**

PLAT340\_ALERT\_3\_B Low Bond Precision on C-C Bonds ..... 0.0114 Ang.  
PLAT911\_ALERT\_3\_B Missing FCF Refl Between Thmin & STh/L= 0.502 2152 Report

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#### **Alert level C**

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C12 --C13 . 0.17 Ang.  
PLAT331\_ALERT\_2\_C Small Aver Phenyl C-C Dist C23 --C28 . 1.37 Ang.  
PLAT767\_ALERT\_4\_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

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#### **Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 15 Note  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 4 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 15 Report  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 15 Note  
PLAT909\_ALERT\_3\_G Percentage of  $I > 2\sigma(I)$  Data at  $\theta(\text{Max})$  Still 100% Note  
PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below  $\theta(\text{Min})$ . 1 Note  
PLAT952\_ALERT\_5\_G Calculated ( $\theta_{\text{Max}}$ ) and CIF-Reported  $I_{\text{max}}$  Differ. 2 Units  
PLAT958\_ALERT\_1\_G Calculated ( $\theta_{\text{Max}}$ ) and Actual (FCF)  $I_{\text{max}}$  Differ. 2 Units  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info

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- 3 **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  
10 **ALERT level G** = General information/check it is not something unexpected

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