

## CHECK CIF FILE of compound 10

### checkCIF/PLATON report

Structure factors have been supplied for datablock(s) db1

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: db1

Bond precision: C-C = 0.0021 Å Wavelength=1.54178

Cell: a=22.9241(2) b=7.3205(1) c=42.5522(4)

alpha=90 beta=90 gamma=90

Temperature: 100 K

Calculated Reported

Volume 7140.94(13) 7140.93(13)

Space group P b c a P b c a

Hall group -P 2ac 2ab -P 2ac 2ab

Moiety formula C24 H34 N6 O4 C24 H34 N6 O4

Sum formula C24 H34 N6 O4 C24 H34 N6 O4

Mr 470.57 470.57

Dx, g cm<sup>-3</sup> 1.313 1.313

Z 12 12

Mu (mm<sup>-1</sup>) 0.745 0.745

F000 3024.0 3024.0

F000' 3033.15

h, k, lmax 27, 8, 51 27, 8, 51

Nref 6534 6453

Tmin, Tmax 0.923, 0.971 0.892, 1.000

Tmin' 0.901

Correction method= # Reported T Limits: Tmin=0.892 Tmax=1.000

AbsCorr = GAUSSIAN

Data completeness= 0.988 Theta(max)= 68.243

R(reflections)= 0.0425( 5944)

wR2(reflections)=

0.1125( 6453)

S = 1.081 Npar= 473

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 C

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for O6 --N9 . 5.2 s.u.

PLAT410\_ALERT\_2\_C Short Intra H...H Contact H1B ..H6 . 1.95 Ang.  
 x,y,z = 1\_555 Check  
 PLAT410\_ALERT\_2\_C Short Intra H...H Contact H2B ..H20 . 1.93 Ang.  
 x,y,z = 1\_555 Check  
 PLAT410\_ALERT\_2\_C Short Intra H...H Contact H3A ..H16 . 1.92 Ang.  
 x,y,z = 1\_555 Check  
 PLAT410\_ALERT\_2\_C Short Intra H...H Contact H4A ..H10 . 1.95 Ang.  
 x,y,z = 1\_555 Check  
 PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 4.468 Check  
 PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 68 Report

#### **Alert level G**

PLAT143\_ALERT\_4\_G s.u. on c - Axis Small or Missing ..... 0.00040 Ang.  
 PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 13 Note  
 PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 4.9 Low  
 PLAT955\_ALERT\_1\_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units  
 PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 8 Info  
 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 5 **ALERT level G** = General information/check it is not something unexpected  
 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 6 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 3 ALERT type 3 Indicator that the structure quality may be low  
 2 ALERT type 4 Improvement, methodology, query or suggestion  
 0 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* 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 18/05/2022; check.def file version of 17/05/2022**

Datablock db1 - ellipsoid plot

