checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ddz20127

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: ddz20127

```
Bond precision:  C-C = 0.0062 A          Wavelength=0.71073

Cell:            a=9.026(2)    b=15.955(4)          c=8.9627(18)
                 alpha=90      beta=115.774(6)      gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	1162.3(5)	1162.3(5)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C32 H28 N2	?
Sum formula	C32 H28 N2	C32 H28 N2
Mr	440.56	440.56
Dx,g cm-3	1.259	1.259
Z	2	2
Mu (mm-1)	0.073	0.073
F000	468.0	468.0
F000’	468.16	
h,k,lmax	10,18,10	10,18,10
Nref	2048	2072
Tmin,Tmax	0.991,0.996	0.557,0.746
Tmin’	0.991	

```
Correction method= # Reported T Limits: Tmin=0.557 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.012          Theta(max)= 24.993

R(reflections)= 0.1040( 1619)     wR2(reflections)= 0.2826( 2072)

S = 1.127                 Npar= 158
```

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

```
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full           ! Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.28 Report
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density       0.56 eA-3
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00618 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595         19 Report
```

Alert level G

```
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        48% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law         [ 1 0-1] Est.d BASF       0.39 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          8 Note
```

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
1 ALERT type 4 Improvement, methodology, query or suggestion
1 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 03/06/2021; check.def file version of 02/06/2021

Datablock ddz20127 - ellipsoid plot