checkCIF/PLATON report

Structure factors have been supplied for datablock(s) vt-33_sq

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: vt-33_sq

```
Bond precision:   C-C = 0.0031 A          Wavelength=0.71073

Cell:             a=18.3186(3)      b=18.3186(3)      c=11.6298(4)
                  alpha=90          beta=90           gamma=90
Temperature:      290 K
```

	Calculated	Reported
Volume	3902.63(18)	3902.62(19)
Space group	P 42/n	P 42/n
Hall group	-P 4bc	-P 4bc
Moiety formula	C15 H12 N4 O4 Zn [+ solvent]	?
Sum formula	C15 H12 N4 O4 Zn [+ solvent]	C15 H12 N4 O4 Zn
Mr	377.68	377.66
Dx,g cm-3	1.286	1.286
Z	8	8
Mu (mm-1)	1.281	1.281
F000	1536.0	1536.0
F000'	1538.84	
h,k,lmax	25,25,15	22,21,15
Nref	5261	4505
Tmin,Tmax	0.926,0.938	0.900,1.000
Tmin'	0.880	

```
Correction method= # Reported T Limits: Tmin=0.900 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.856          Theta(max)= 29.164
```

R(reflections)= 0.0358(3519)

wR2(reflections)= 0.0965(4505)

S = 1.047 Npar= 267

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

PLAT215_ALERT_3_C Disordered C101 has ADP max/min Ratio ..... 3.8 Note
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Zn1 Check

---

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Zn1 --O1 . 13.0 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of N1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N101 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N102 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N202 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C101 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C102 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C201 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C202 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C203 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C301 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C401 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H13B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H102 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H201 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H202 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H203 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H301 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H401 Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 23% Note
PLAT411_ALERT_2_G Short Inter H...H Contact H9 ..H203 . 2.13 Ang.
1/2-y,x,3/2-z = 8_657 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 554 A**3
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 19 Check
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers 1 Check
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 596 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.9 Low
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 3 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 4 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

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

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  4 ALERT type 3 Indicator that the structure quality may be low
 27 ALERT type 4 Improvement, methodology, query or suggestion
  3 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 10/05/2023; check.def file version of 10/05/2023

Datablock vt-33_sq - ellipsoid plot