

## checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: ad47

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Bond precision:    C-C = 0.0055 A                      Wavelength=0.71073

Cell:                      a=16.320(4)              b=16.320(4)              c=12.476(3)  
                                    alpha=90              beta=90              gamma=120  
Temperature:              293 K

	Calculated	Reported
Volume	2877.7(18)	2877.7(12)
Space group	P -3	P -3
Hall group	-P 3	?
Moiety formula	3(C28 H40 Cu2 N8 O2), 2(Er H6 N3 O12)	?
Sum formula	C84 H132 Cu6 Er2 N30 O30	C42 H66 Cu3 Er N15 O15
Mr	2758.02	1378.98
Dx, g cm <sup>-3</sup>	1.592	1.591
Z	1	2
Mu (mm <sup>-1</sup> )	2.609	2.609
F000	1396.0	1396.0
F000'	1397.89	
h,k,lmax	20,20,15	20,20,15
Nref	4185	4184
Tmin,Tmax	0.348,0.770	0.705,1.000
Tmin'	0.261	

Correction method= # Reported T Limits: Tmin=0.705 Tmax=1.000  
AbsCorr = PSI-SCANS

Data completeness= 1.000                      Theta(max)= 26.970

R(reflections)= 0.0277( 3304)              wR2(reflections)= 0.0699( 4184)

S = 1.126                      Npar= 237

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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**

PLAT601\_ALERT\_2\_A Structure Contains Solvent Accessible VOIDS of . 290 Ang\*\*3

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**Alert level B**

PLAT415\_ALERT\_2\_B Short Inter D-H..H-X H2O5 ..H14A .. 1.95 Ang.

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**Alert level C**

WEIGH01\_ALERT\_1\_C Extra text has been found in the  
\_refine\_ls\_weighting\_scheme field. This should be in the  
\_refine\_ls\_weighting\_details field.

Weighting scheme given as calc w=1/[\s^2^(Fo^2^)+(0.0283P)^2^+1.4604

Weighting scheme identified as calc

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for O2 --N5 . 6.0 s.u.

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Er Check

PLAT250\_ALERT\_2\_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.4 Note

PLAT412\_ALERT\_2\_C Short Intra XH3 .. XHn H8B ..H13A .. 1.82 Ang.

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**Alert level G**

ABSTY01\_ALERT\_1\_G Extra text has been found in the \_exptl\_absorpt\_correction\_type  
field, which should be only a single keyword. A literature  
citation should be included in the \_exptl\_absorpt\_process\_details  
field.

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 3 Note

PLAT005\_ALERT\_5\_G No Embedded Refinement Details Found in the CIF Please Do !

PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.50 Check

PLAT152\_ALERT\_1\_G The Supplied and Calc. Volume s.u. Differ by ... 6 Units

PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature ..... (K) 293 Check

PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature ..... (K) 293 Check

PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Er --O3 . 5.8 s.u.

PLAT380\_ALERT\_4\_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C13 Check

PLAT380\_ALERT\_4\_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C14 Check

PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 2 Note

PLAT808\_ALERT\_5\_G No Parseable SHELXL Style Weighting Scheme Found Please Check

PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL 2016 Note

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- 1 **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  
13 **ALERT level G** = General information/check it is not something unexpected

- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 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
-

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.

### Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_WEIGH01_ad47
;
PROBLEM: Extra text has been found in the
RESPONSE: ...
;
_vrf_PLAT601_ad47
;
PROBLEM: Structure Contains Solvent Accessible VOIDS of .          290 Ang**3
RESPONSE: ...
;
_vrf_PLAT230_ad47
;
PROBLEM: Hirshfeld Test Diff for  O2      --N5      .          6.0 s.u.
RESPONSE: ...
;
_vrf_PLAT241_ad47
;
PROBLEM: High  'MainMol' Ueq as Compared to Neighbors of          01 Check
RESPONSE: ...
;
_vrf_PLAT242_ad47
;
PROBLEM: Low   'MainMol' Ueq as Compared to Neighbors of          Er Check
RESPONSE: ...
;
_vrf_PLAT250_ad47
```

```

;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.4 Note
RESPONSE: ...
;
_vrf_PLAT412_ad47
;
PROBLEM: Short Intra XH3 .. XHn   H8B   ..H13A   ..      1.82 Ang.
RESPONSE: ...
;
# end Validation Reply Form

```

**PLATON version of 13/08/2017; check.def file version of 12/12/2017**

Datablock ad47 - ellipsoid plot

