

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) u16_01

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: u16_01

Bond precision: C-C = 0.0040 A

Wavelength=0.71073

Cell: a=13.8689(18) b=14.0995(18) c=14.6916(19)
 alpha=112.944(2) beta=96.288(2) gamma=112.879(2)
Temperature: 100 K

	Calculated	Reported
Volume	2319.2(5)	2319.2(5)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C34 H52 Cu2 N12, 2(C F3 O3 S)	C34 H52 Cu2 N12, 2(C F3 O3 S)
Sum formula	C36 H52 Cu2 F6 N12 O6 S2	C36 H52 Cu2 F6 N12 O6 S2
Mr	1054.12	1054.10
Dx,g cm-3	1.510	1.509
Z	2	2
Mu (mm-1)	1.087	1.087
F000	1088.0	1088.0
F000'	1090.25	
h,k,lmax	18,19,19	18,19,19
Nref	12192	12115
Tmin,Tmax	0.729,0.770	0.709,0.780
Tmin'	0.684	

Correction method= # Reported T Limits: Tmin=0.709 Tmax=0.780

AbsCorr = MULTI-SCAN

Data completeness= 0.994

Theta(max)= 28.890

R(reflections)= 0.0446(8955)

wR2(reflections)= 0.1092(12115)

S = 1.010

Npar= 585

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

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S2 Check



Alert level G

PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) S2 -- C36 .. 5.2 s.u.
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C35 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C36 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in Structure ... 149 A**3
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed ! Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
7 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 19/11/2015; check.def file version of 17/11/2015

