

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mfr200008\_tw\_twin1\_hklf4

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: mfr200008\_tw\_twin1\_hklf4

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Bond precision:    C-C = 0.0117 Å                      Wavelength=1.54184

Cell:                      a=14.5781(2)              b=26.2433(4)              c=26.0188(3)  
                            alpha=90                      beta=103.544(1)              gamma=90  
Temperature:              150 K

	Calculated	Reported
Volume	9677.4(2)	9677.4(2)
Space group	C c	C 1 c 1
Hall group	C -2yc	C -2yc
Moiety formula	C36 H36 Cu2 N8, 2(C2 F6 N O4 S2)	C36 H36 Cu2 N8, 2(C2 F6 N O4 S2)
Sum formula	C40 H36 Cu2 F12 N10 O8 S4	C40 H36 Cu2 F12 N10 O8 S4
Mr	1268.13	1268.11
Dx,g cm-3	1.741	1.741
Z	8	8
Mu (mm-1)	3.685	3.685
F000	5120.0	5120.0
F000'	5116.74	
h,k,lmax	17,31,31	17,31,30
Nref	17167[ 8591]	19482
Tmin,Tmax	0.541,0.802	0.973,0.990
Tmin'	0.491	

Correction method= # Reported T Limits: Tmin=0.973 Tmax=0.990  
AbsCorr = ANALYTICAL

Data completeness= 2.27/1.13                      Theta(max)= 66.801

R(reflections)= 0.0431( 18477)                      wR2(reflections)= 0.1170( 19482)

S = 1.033                                      Npar= 1370

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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 C**

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18) .....	6.25	Note
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C38	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C56	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S5	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S6	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.01169	Ang.
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of .	31	Ang**3
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.596	28	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1	Check

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**Alert level G**

PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C73	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C74	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C75	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C76	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C77	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C78	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C79	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C80	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F12 ..F20	2.81	Ang.
	x,y,z =	1_555	Check
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	90%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT916_ALERT_2_G	Hooft y and Flack x Parameter Values Differ by .	0.27	Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law ( 0 0 1) Est.d BASF	0.42	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	4	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	2.3	Low

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
16 ALERT type 2 Indicator that the structure model may be wrong or deficient  
7 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

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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.

