checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mfr200004

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: mfr200004

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Bond precision:  C-C = 0.0054 A          Wavelength=0.68890

Cell:          a=8.3285(8)        b=14.6788(15)     c=15.9531(16)
               alpha=113.555(2)   beta=100.232(2)   gamma=99.398(2)
Temperature:   100 K
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	Calculated	Reported
Volume	1699.0(3)	1699.0(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C18 H14 Cu F6 N5 O4 S4, C2 F6 N O4 S2	C18 H14 Cu F6 N5 O4 S4, C2 F6 N O4 S2
Sum formula	C20 H14 Cu F12 N6 O8 S6	C20 H14 Cu F12 N6 O8 S6
Mr	950.28	950.27
Dx,g cm-3	1.858	1.858
Z	2	2
Mu (mm-1)	1.031	1.042
F000	946.0	946.0
F000’	948.68	
h,k,lmax	10,19,20	10,19,20
Nref	7789	7697
Tmin,Tmax		0.426,0.746
Tmin’		

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Correction method= # Reported T Limits: Tmin=0.426 Tmax=0.746
AbsCorr = NONE

Data completeness= 0.988          Theta(max)= 26.571

R(reflections)= 0.0595( 6160)     wR2(reflections)= 0.1721( 7697)

S = 1.097                 Npar= 478
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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.

Alert level C

PLAT214_ALERT_2_C Atom F11 (Anion/Solvent) ADP max/min Ratio 4.1 prolat
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S6 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.4 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.9 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 61 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.84A From Cu1 1.51 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.68890 Ang.
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C18 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C20 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (I) . 1.36 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 443 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 31 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info
PLAT984_ALERT_1_G The Cu-f'= 0.2709 Deviates from the B&C-Value 0.3307 Check
PLAT984_ALERT_1_G The F-f'= 0.0124 Deviates from the B&C-Value 0.0164 Check
PLAT984_ALERT_1_G The N-f'= 0.0037 Deviates from the B&C-Value 0.0056 Check
PLAT984_ALERT_1_G The O-f'= 0.0071 Deviates from the B&C-Value 0.0101 Check
PLAT984_ALERT_1_G The S-f'= 0.1048 Deviates from the B&C-Value 0.1187 Check

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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
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
19 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 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.

PLATON version of 05/12/2020; check.def file version of 05/12/2020

Datablock mfr200004 - ellipsoid plot