checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 82554772_shelxt

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: 82554772_shelxt

Bond precision: C-C = 0.0048 A Wavelength=0.68890

Cell: a=8.77390(11) b=10.90700(13) c=17.79310(19)
alpha=90 beta=102.174(1) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1664.45(3)	1664.45(3)
Space group	P n	P 1 n 1
Hall group	P -2yac	P -2yac
Moiety formula	C20 H18 Cu F6 N5 O4 S2, C2 F6 N O4 S2	C18 H18 Cu N4, 2(C2 F6 N O4 S2)
Sum formula	C22 H18 Cu F12 N6 O8 S4	C22 H18 Cu F12 N6 O8 S4
Mr	914.21	914.20
Dx,g cm-3	1.824	1.824
Z	2	2
Mu (mm-1)	0.940	0.949
F000	914.0	914.0
F000’	916.21	
h,k,lmax	11,14,23	11,14,23
Nref	7646[3830]	7453
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 1.95/0.97 Theta(max)= 26.572

R(reflections)= 0.0276(7233) wR2(reflections)= 0.0706(7453)

S = 1.039 Npar= 523

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

```
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       7.31 Note
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S4 Check
PLAT431_ALERT_2_C Short Inter HL..A Contact  F1       ..O5       .       2.78 Ang.
                                                  x,1+y,z  =      1_565 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          2 Report
```

Alert level G

```
ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         12 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         58 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.68890 Ang.
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         11 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =          3 Note
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        C19 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C21 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17A       Constrained at     0.5294 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17B       Constrained at     0.4706 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16C       Constrained at     0.5294 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16D       Constrained at     0.5294 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17C       Constrained at     0.5294 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17D       Constrained at     0.5294 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18C       Constrained at     0.5294 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18D       Constrained at     0.5294 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16A       Constrained at     0.4706 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H16B       Constrained at     0.4706 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17A       Constrained at     0.4706 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17B       Constrained at     0.4706 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18A       Constrained at     0.4706 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18B       Constrained at     0.4706 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F10A       Constrained at     0.5914 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F11A       Constrained at     0.5914 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F12A       Constrained at     0.5914 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F10B       Constrained at     0.4086 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F11B       Constrained at     0.4086 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F12B       Constrained at     0.4086 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22A       Constrained at     0.5914 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22B       Constrained at     0.4086 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )          3% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )         27% Note
PLAT434_ALERT_2_G Short Inter HL..HL Contact F4       ..F12A            2.76 Ang.
                                                 -1+x,y,z  =      1_455 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F4       ..F12B            2.82 Ang.
                                                 -1+x,y,z  =      1_455 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F5       ..F7              2.84 Ang.
                                      -1/2+x,-2-y,-1/2+z  =      2_434 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        614 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          7 Info
PLAT984_ALERT_1_G The Cu-f'=    0.3483 Deviates from the B&C-Value     0.3307 Check
PLAT985_ALERT_1_G The Cu-f"=    1.2194 Deviates from the B&C-Value     1.2021 Check
```

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

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 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
 29 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 05/12/2020; check.def file version of 05/12/2020

Datablock 82554772_shelxt - ellipsoid plot