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: I

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Bond precision:  C-C = 0.0100 A          Wavelength=0.71073

Cell:          a=12.0582(3)      b=12.9571(4)     c=14.6191(4)
               alpha=78.873(2)   beta=74.229(3)   gamma=69.542(2)
Temperature:   296 K
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	Calculated	Reported
Volume	2047.26(11)	2047.26(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H34 Cu2 F4 N2 O8	C42 H34 Cu2 F4 N2 O8
Sum formula	C42 H34 Cu2 F4 N2 O8	C42 H34 Cu2 F4 N2 O8
Mr	897.81	897.79
Dx,g cm-3	1.457	1.456
Z	2	2
Mu (mm-1)	1.111	1.111
F000	916.0	916.0
F000’	917.74	
h,k,lmax	14,15,17	14,15,17
Nref	7432	7330
Tmin,Tmax	0.808,0.846	0.738,0.785
Tmin’	0.717	

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Correction method= # Reported T Limits: Tmin=0.738 Tmax=0.785
AbsCorr = MULTI-SCAN

Data completeness= 0.986          Theta(max)= 25.250

R(reflections)= 0.0482( 3517)     wR2(reflections)= 0.1103( 7330)

S = 0.988                 Npar= 531
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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

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PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..         48 %
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O3     --  C9      ..        5.5 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C26 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C28 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C11 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C14 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C22 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C24 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C27 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C32 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C35 Check
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C11    -C16          1.37 Ang.
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C32    -C37          1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01003 Ang.
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Alert level G

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PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of *C2A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C2B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C23A   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C23B   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2C    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H2D    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23A   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23B   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23C   is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *H23D   is Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1)..          3 % Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C9     Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C30    Check
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C9     -   C10    ..       1.50 Ang.
PLAT367_ALERT_2_G Long?   C(sp?)-C(sp?) Bond  C30    -   C31    ..       1.51 Ang.
PLAT607_ALERT_4_G ADDSYM Test Skipped due to severe Disorder .....          ! Info
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         38 Check
              C2A  -C1   -C2B     1.555   1.555   1.555             16.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         48 Check
              C2A  -C3   -C2B     1.555   1.555   1.555             17.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         85 Check
              C2B  -C2A  -H2C     1.555   1.555   1.555             14.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #         92 Check
              H2A  -C2A  -H2C     1.555   1.555   1.555             39.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        100 Check
              C2A  -C2B  -H2B     1.555   1.555   1.555             14.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        111 Check
              H2B  -C2B  -H2D     1.555   1.555   1.555             38.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        151 Check
              C23A -C22  -C23B    1.555   1.555   1.555             11.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        158 Check
              C23A -C24  -C23B    1.555   1.555   1.555             11.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        196 Check
              C23B -C23A -H23C    1.555   1.555   1.555             20.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        203 Check
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              H23A -C23A -H23C    1.555   1.555   1.555             26.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        206 Check
              H23B -C23A -H23D    1.555   1.555   1.555             36.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        213 Check
              C23A -C23B -H23B    1.555   1.555   1.555             20.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        221 Check
              H23A -C23B -H23C    1.555   1.555   1.555             35.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        224 Check
              H23B -C23B -H23D    1.555   1.555   1.555             26.00 Deg.
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #         98 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         8 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
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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
  18 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  37 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  20 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
  31 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 24/11/2016; check.def file version of 23/11/2016

Datablock I - ellipsoid plot