checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) kaoh503

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
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: kaoh503

Bond precision: C-C = 0.0018 A Wavelength=0.71073
Cell: a=9.2626(8) b=9.5087(8) c=11.0617(9)
alpha=89.565(2) beta=76.519(2) gamma=67.742(2)
Temperature: 100 K

	Calculated	Reported
Volume	873.29(13)	873.29(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C12 H18 Cl Cu N5 O2 S, 2(H2 O)	(C12 H18 Cl Cu N5 O2 S), 2(H2 O)
Sum formula	C12 H22 Cl Cu N5 O4 S	C12 H22 Cl Cu N5 O4 S
Mr	431.41	431.39
Dx,g cm-3	1.641	1.641
Z	2	2
Mu (mm-1)	1.550	1.550
F000	446.0	446.0
F000'	447.32	
h,k,lmax	13,13,15	13,13,15
Nref	5210	5185
Tmin,Tmax	0.671,0.711	0.653,0.727
Tmin'	0.622	

Correction method= # Reported T Limits: Tmin=0.653 Tmax=0.727 AbsCorr = MULTI-SCAN
Data completeness= 0.995 Theta(max)= 30.262
R(reflections)= 0.0215(4859) wR2(reflections)= 0.0577(5185)
S = 1.062 Npar= 223

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

PLAT480_ALERT_4_C Long H...A H-Bond Reported H1 ..CL 2.87 Ang.
And 2 other PLAT480 Alerts

PLAT480_ALERT_4_C Long H...A H-Bond Reported H10A ..CL 2.90 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H11B ..O2 2.62 Ang.

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PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          5 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          4 Note
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Alert level G

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PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          8 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.002 Degree
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu       --Cl        .        7.5 s.u.
And 2 other PLAT232 Alerts

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu       --S         .       10.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu       --O2        .       17.0 s.u.

PLAT794_ALERT_5_G Tentative Bond Valency for Cu        (II)      .       2.23 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         21 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.          8 Info
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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
  5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 11 ALERT level G = General information/check it is not something unexpected

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  5 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
  4 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

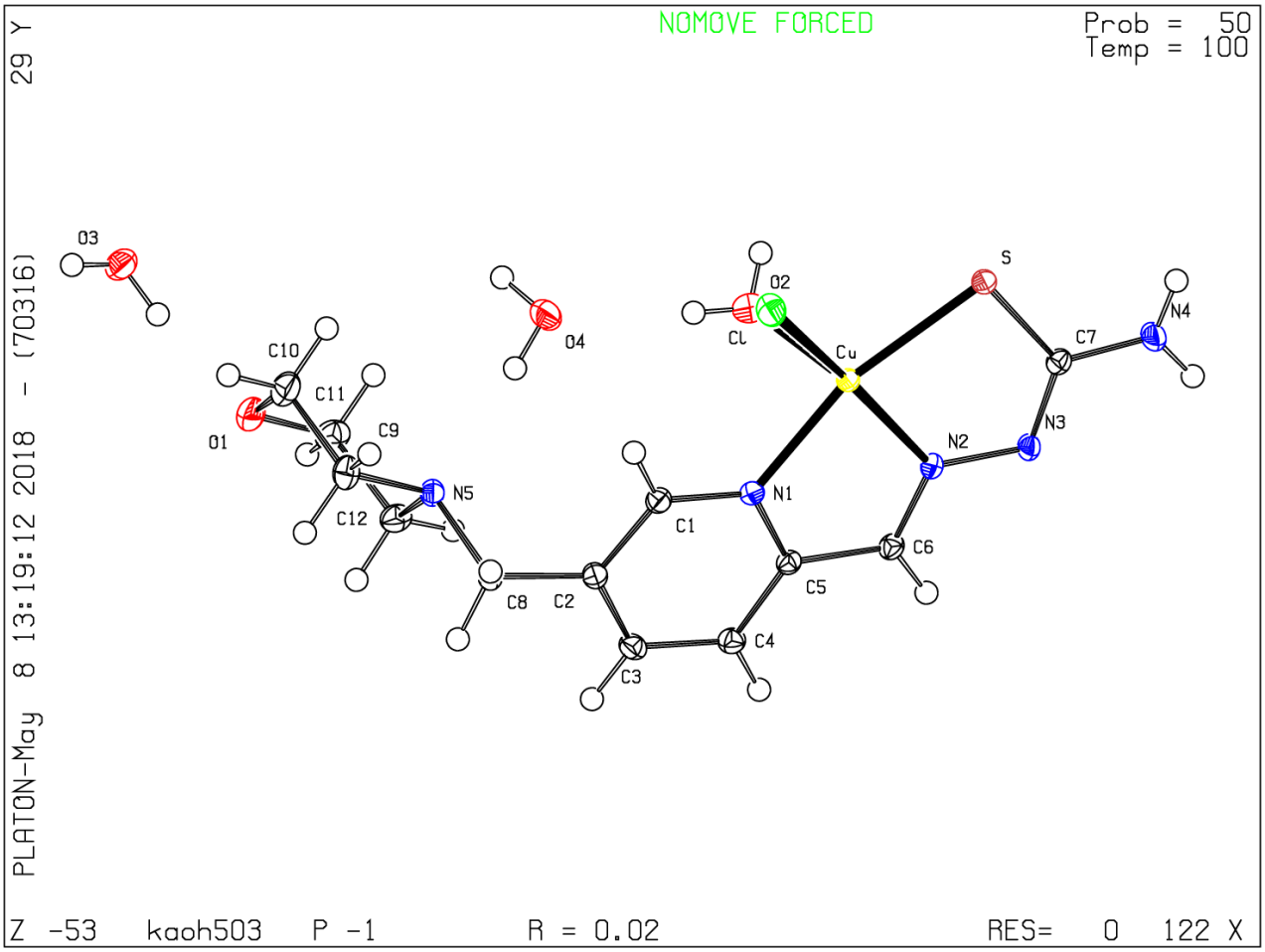
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 23/04/2018; check.def file version of 23/04/2018

Datablock kaoh503 - ellipsoid plot



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Test a new CIF entry