checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1, 1.solv, 2, 3

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: 1

Bond precision: N- C = 0.0060 A Wavelength=0.71073

Cell: a=6.6586(7) b=12.8635(14) c=17.4187(19)
alpha=90 beta=99.657(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1470.8(3)	1470.8(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C10 H20 Cl6 Cu3 N16 O2 S4	C10 H20 Cl6 Cu3 N16 O2 S4
Sum formula	C10 H20 Cl6 Cu3 N16 O2 S4	C10 H20 Cl6 Cu3 N16 O2 S4
Mr	928.01	927.98
Dx,g cm-3	2.095	2.095
Z	2	2
Mu (mm-1)	3.024	3.024
F000	922.0	922.0
F000’	926.79	
h,k,lmax	8,17,23	8,17,23
Nref	3696	3688
Tmin,Tmax	0.920,0.938	0.642,0.746
Tmin’	0.683	

Correction method= # Reported T Limits: Tmin=0.642 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 28.434

R(reflections)= 0.0494(2997) wR2(reflections)= 0.1130(3688)

S = 1.143 Npar= 197

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 B

```
PLAT431_ALERT_2_B Short Inter HL..A Contact  Cl2      ..S1       .       3.09 Ang.
                                          1-x,1-y,1-z  =      3_666 Check
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ...          1 Check
```

Alert level C

```
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        7.5 Ratio
PLAT480_ALERT_4_C Long H...A H-Bond Reported H12A     ..S2       .       2.90 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H12A     ..N6       .       2.68 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1D      ..CL3      .       2.86 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1A      ..CL1      .       2.93 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      5.403 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....          1 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.92A   From N6             0.70 eA-3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       6.01 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.07 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2       (II)      .       2.05 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          2 Note
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          6 Note
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
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  10 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
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Datablock: 1.solv

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Bond precision:  C-C = 0.0025 A          Wavelength=0.71073

Cell:          a=6.7181(5)       b=12.9961(9)     c=12.9971(9)
               alpha=64.067(2)   beta=79.492(2)   gamma=82.134(2)
Temperature:   100 K
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	Calculated	Reported
Volume	1001.29(12)	1001.29(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C10 H20 Cl6 Cu3 N16 O2 S4, 4(C2 H3 N)	C10 H20 Cl6 Cu3 N16 O2 S4, 4(C2 H3 N)
Sum formula	C18 H32 Cl6 Cu3 N20 O2 S4	C18 H32 Cl6 Cu3 N20 O2 S4
Mr	1092.23	1092.19
Dx,g cm-3	1.811	1.811
Z	1	1
Mu (mm-1)	2.239	2.239
F000	549.0	549.0
F000’	551.41	
h,k,lmax	9,18,18	9,18,18
Nref	6166	6158
Tmin,Tmax	0.734,0.853	0.613,0.746
Tmin’	0.542	

Correction method= # Reported T Limits: Tmin=0.613 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 30.576

R(reflections)= 0.0209(5643) wR2(reflections)= 0.0514(6158)

S = 1.079 Npar= 246

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	H1A	..S2	.	2.94 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported	H1B	..CL2	.	2.95 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported	H1B	..S1	.	2.95 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported	H22B	..N31	.	2.68 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported	H12C	..CL3	.	2.95 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported	H31A	..N2	.	2.64 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported	H31C	..CL1	.	2.98 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported	H1C	..CL1	.	2.99 Ang.
PLAT976_ALERT_2_C Check Calcd Resid. Dens.	0.98A	From O1		-0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on	H1C			-0.44 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on	H1D			-0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on	H31B			-0.39 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension				1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms				2 Report
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)	Cu1	--N8_c	.	6.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)	Cu2	--Cl1	.	8.1 s.u.

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PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cu2      --O1       .       5.8 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .      2.10 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2       (II)      .      2.10 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         5 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.         1 Info
```

```
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   4 ALERT type 5 Informative message, check
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Datablock: 2

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Bond precision:  C-C = 0.0020 A          Wavelength=0.71073

Cell:            a=10.1237(5)    b=9.5414(5)        c=14.4784(8)
                 alpha=90        beta=93.650(2)     gamma=90
Temperature:     100 K
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	Calculated	Reported
Volume	1395.69(13)	1395.69(13)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C12 H20 Cl4 Cu4 N16 S4	C12 H20 Cl4 Cu4 N16 S4
Sum formula	C12 H20 Cl4 Cu4 N16 S4	C12 H20 Cl4 Cu4 N16 S4
Mr	912.68	912.64
Dx,g cm-3	2.172	2.172
Z	2	2
Mu (mm-1)	3.729	3.729
F000	904.0	904.0
F000’	908.80	
h,k,lmax	13,12,19	13,12,19
Nref	3490	3486
Tmin,Tmax	0.439,0.827	0.484,0.746
Tmin’	0.214	

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Correction method= # Reported T Limits: Tmin=0.484 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 28.339
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R(reflections)= 0.0212(3181) wR2(reflections)= 0.0480(3486)

S = 1.081 Npar= 183

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

PLAT431_ALERT_2_C Short Inter HL..A Contact Cl2 ..S2 . 3.34 Ang.
-1/2+x,3/2-y,-1/2+z = 4_575 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H2A ..N4 . 2.69 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1B ..CL2 . 2.84 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H1B ..CL1 . 2.85 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H12B ..S2 . 2.95 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H12C ..CL2 . 2.87 Ang.

Alert level G

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 --Cl1 . 7.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 --Cl2_a . 22.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu2 --Cl1 . 35.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu2 --Cl1_a . 62.0 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact N2 ..C21 2.98 Ang.
1-x,1-y,1-z = 3_666 Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 4 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. 1 Info

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0 ALERT type 3 Indicator that the structure quality may be low
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0 ALERT type 5 Informative message, check

Datablock: 3

Bond precision: C-C = 0.0020 A Wavelength=0.71073

Cell: a=20.3164(18) b=6.5444(6) c=12.8543(11)
alpha=90 beta=109.493(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1611.1(2)	1611.1(2)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C3 H5 Cl2 Cu N4 S	C3 H5 Cl2 Cu N4 S
Sum formula	C3 H5 Cl2 Cu N4 S	C3 H5 Cl2 Cu N4 S
Mr	263.62	263.61
Dx,g cm-3	2.174	2.174
Z	8	8
Mu (mm-1)	3.567	3.567
F000	1040.0	1040.0
F000'	1046.00	
h,k,lmax	26,8,17	26,8,17
Nref	2020	2015
Tmin,Tmax	0.804,0.852	0.702,0.746
Tmin'	0.776	

Correction method= # Reported T Limits: Tmin=0.702 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 28.354

R(reflections)= 0.0196(1899) wR2(reflections)= 0.0461(2015)

S = 1.166 Npar= 101

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

PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

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Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/c I2/a Note
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu --Cl1 . 5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu --N2 . 6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu --Cl1_b . 6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu --Cl2_c . 6.3 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact N4 ..C12 2.96 Ang.
x,-1+y,z = 1_545 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl1 ..Cl2 3.40 Ang.
x,1+y,z = 1_565 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu (II) . 1.92 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 4 Note

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```
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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

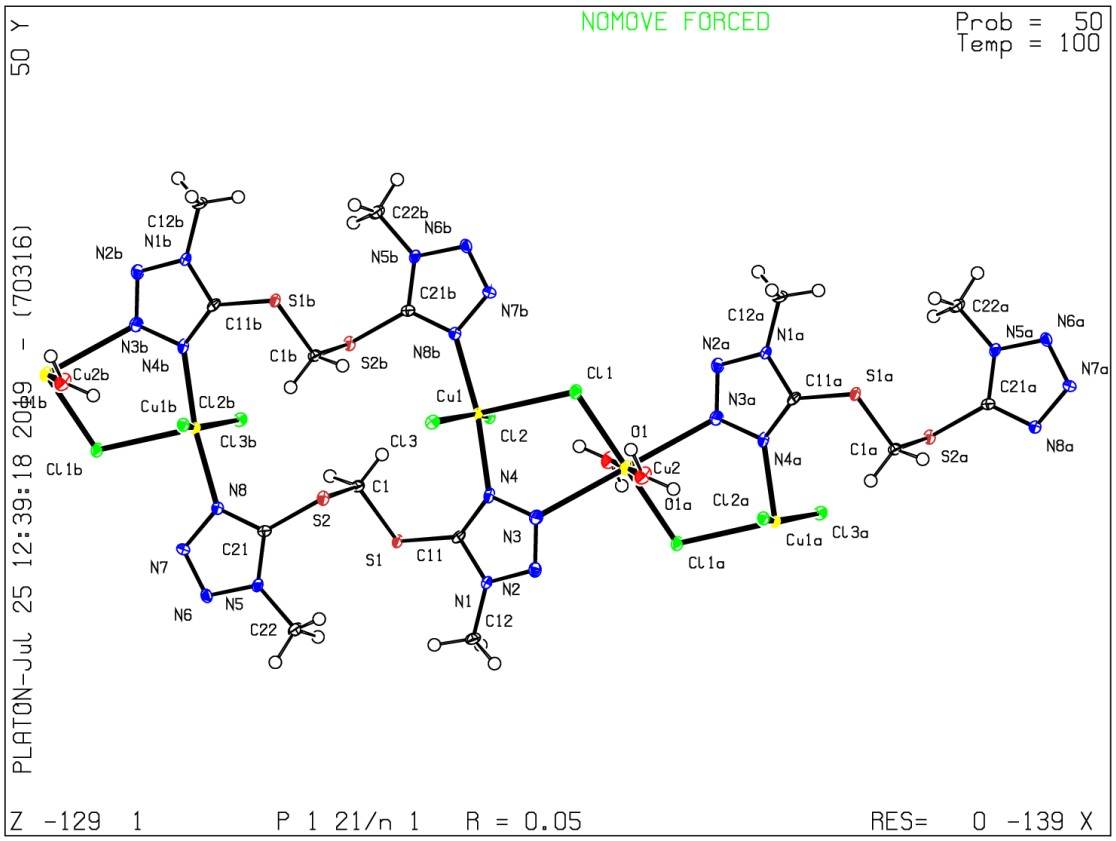
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

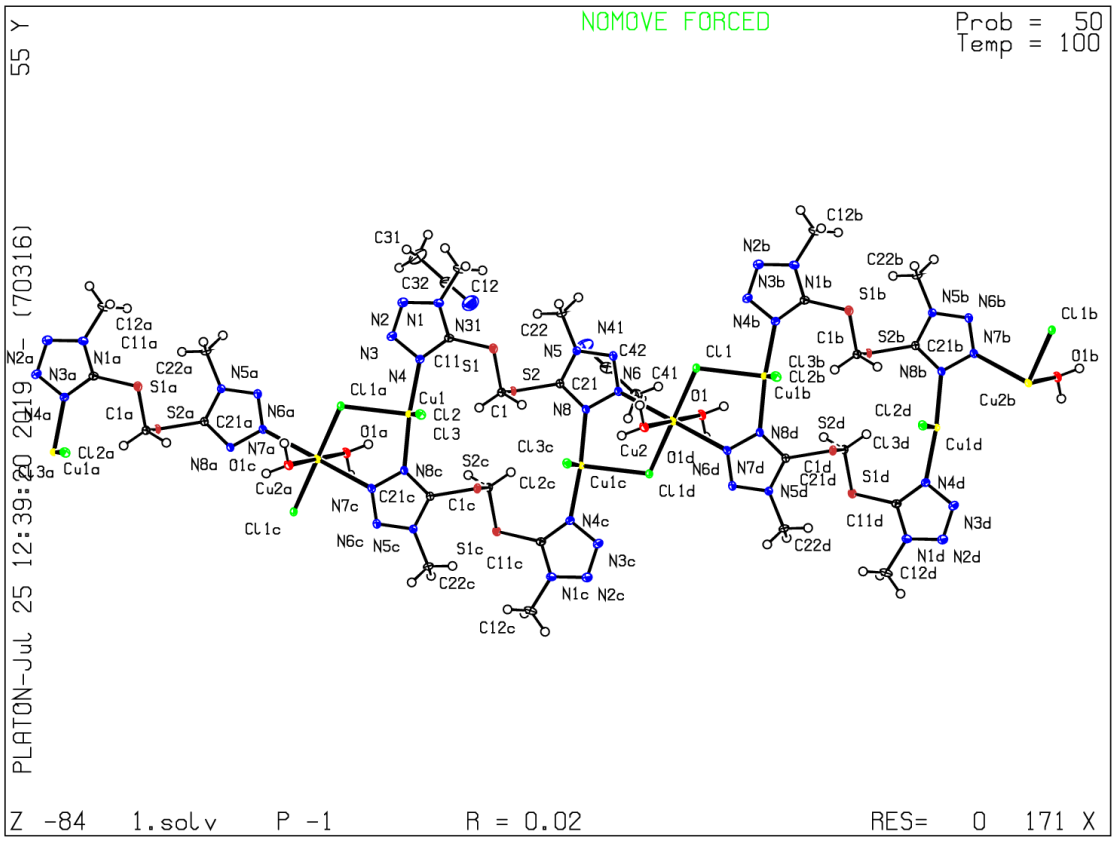
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

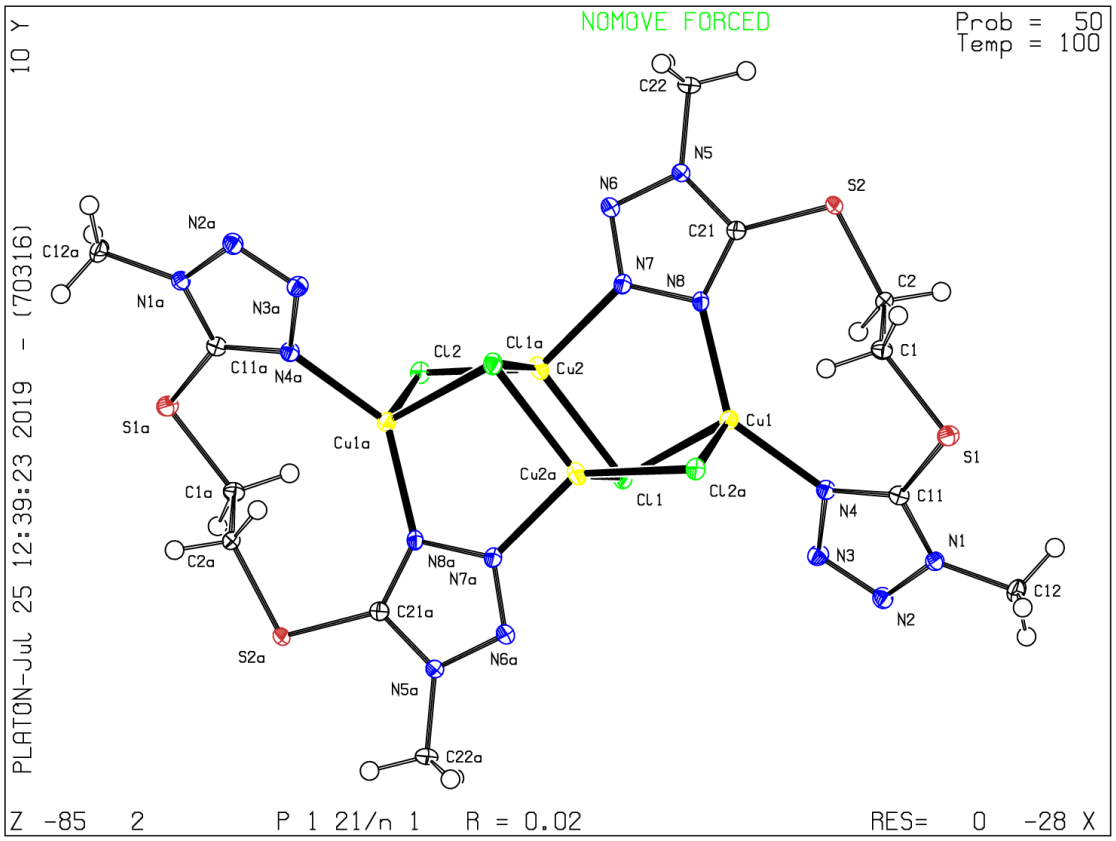
Datablock 1 - ellipsoid plot



Datablock 1.solv - ellipsoid plot



Datablock 2 - ellipsoid plot



Datablock 3 - ellipsoid plot