checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CuL1Cl-MeOH, CuL3Cl-H2O, L2, L2-H2O, L3

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: L2-H2O

Bond precision: C-C = 0.0017 A Wavelength=1.54184

Cell: a=30.9433(6) b=7.1495(2) c=12.1772(2)
alpha=90 beta=93.864(2) gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	2687.83(10)	2687.83(10)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C13 H10 Cl2 N4 O), H2 O	2(C13 H10 Cl2 N4 O), H2 O
Sum formula	C26 H22 Cl4 N8 O3	C26 H22 Cl4 N8 O3
Mr	636.32	636.31
Dx,g cm-3	1.572	1.572
Z	4	4
Mu (mm-1)	4.406	4.406
F000	1304.0	1304.0
F000'	1313.10	
h,k,lmax	38,8,15	38,8,15
Nref	2668	2649
Tmin,Tmax	0.557,0.703	0.327,1.000
Tmin'	0.187	

Correction method= # Reported T Limits: Tmin=0.327 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.993 Theta(max)= 72.523

R(reflections)= 0.0251(2493) wR2(reflections)= 0.0682(2649)

S = 1.077 Npar= 198

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

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
-15 1 1, -2 2 1,

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 3 Report
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl19 ..Cl20 . 3.36 Ang.
1/2+x,3/2-y,1/2+z = 8_566 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 4 Note
PLAT910_ALERT_3_G Missing FCF Reflection(s) Below Theta(Min)[Deg]= 5.73 Note
2 0 0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 16 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
-2 2 1,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
-15 1 1, -2 2 1,
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by . 1 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 4.349 Note
Predicted wR2: Based on SigI**2 1.57 or SHELX Weight 6.33 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 12 Info

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12 **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
4 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: L3

Bond precision: C-C = 0.0055 A Wavelength=1.54184

Cell:	a=5.0471(1)	b=11.7552(3)	c=23.1569(6)
	alpha=90	beta=90	gamma=90
Temperature:	120 K		

	Calculated	Reported
Volume	1373.89(6)	1373.89(6)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C14 H13 Cl N4 O2	C14 H13 Cl N4 O2
Sum formula	C14 H13 Cl N4 O2	C14 H13 Cl N4 O2
Mr	304.73	304.73
Dx,g cm-3	1.473	1.473
Z	4	4
Mu (mm-1)	2.564	2.564
F000	632.0	632.0
F000'	635.24	
h,k,lmax	6,14,29	6,14,29
Nref	2864[1699]	2521
Tmin,Tmax	0.871,0.972	0.648,1.000
Tmin'	0.494	

Correction method= # Reported T Limits: Tmin=0.648 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 1.48/0.88 Theta(max)= 75.776

R(reflections)= 0.0474(2338) wR2(reflections)= 0.1376(2521)

S = 1.081 Npar= 200

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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.972 Why?
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.22 Report
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0055 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 42 Report

6	0	0,	6	1	0,	1	13	0,	6	0	1,	6	1	1,	6	0	2,
0	2	3,	5	7	4,	1	10	6,	5	0	7,	0	9	7,	5	0	8,
5	1	8,	0	7	8,	3	0	9,	0	11	9,	0	11	11,	0	10	14,
0	10	15,	1	4	16,	0	11	16,	3	6	18,	3	0	19,	3	1	19,
3	2	19,	0	4	19,	4	4	19,	3	0	20,	3	1	20,	3	2	20,

(12 More NOT listed: see .ckf listing file)

PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage 80 %

Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          5 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          2 Report
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         66 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          4 Note
               -2  1 26,  -2 11 14,   2  0 26,   2  1 26,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.1 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      2.637 Note
             Predicted wR2: Based on SigI**2  5.22 or SHELX Weight 12.73 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
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1 ALERT type 5 Informative message, check

Datablock: CuL1Cl-MeOH

Bond precision: C-C = 0.0077 A Wavelength=1.54184

Cell:	a=11.7162(6)	b=15.3768(8)	c=17.7976(11)
	alpha=90	beta=97.510(6)	gamma=90
Temperature:	120 K		

	Calculated	Reported
Volume	3178.9(3)	3178.9(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H10 Cl2 Cu N4 O, C H4 O	C13 H10 Cl2 Cu N4 O, C H4 O
Sum formula	C14 H14 Cl2 Cu N4 O2	C14 H14 Cl2 Cu N4 O2
Mr	404.74	404.73
Dx,g cm-3	1.691	1.691
Z	8	8
Mu (mm-1)	5.163	5.164
F000	1640.0	1640.0
F000'	1633.63	
h,k,lmax	14,19,22	14,18,21
Nref	6316	6120
Tmin,Tmax	0.856,0.955	0.616,1.000
Tmin'	0.335	

Correction method= # Reported T Limits: Tmin=0.616 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.969 Theta(max)= 72.729

R(reflections)= 0.0669(4397) wR2(reflections)= 0.1736(6120)

S = 1.015 Npar= 435

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

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00767 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 4.375 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 13 Report
1 9 1, -14 0 2, 0 0 2, -14 1 2, -14 1 3, 6 3 3,
-14 0 4, -14 1 4, -9 14 4, -1 18 4, 6 9 9, 0 3 10,
-8 6 17,

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 12 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 6 Note
H2SA H2SB H2SC H4SA H4SB H4SC
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 6 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 178 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note

```
               6  9  9,   0  3 10,   1  9  1,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....        2.2 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      1.436 Note
             Predicted wR2: Based on SigI**2 12.09 or SHELX Weight 17.10 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  10 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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Datablock: CuL3Cl-H2O

Bond precision: C-C = 0.0027 A Wavelength=1.54184

Cell: a=15.8038(1) b=13.2883(1) c=30.9004(2)
alpha=90 beta=90 gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	6489.26(8)	6489.26(8)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C14 H12 Cl2 Cu N4 O2, H2 O	H2 O, C14 H12 Cl2 Cu N4 O2
Sum formula	C14 H14 Cl2 Cu N4 O3	C14 H14 Cl2 Cu N4 O3
Mr	420.74	420.73
Dx,g cm-3	1.723	1.723
Z	16	16
Mu (mm-1)	5.134	5.134
F000	3408.0	3408.0
F000'	3396.04	
h,k,lmax	19,16,38	19,16,38
Nref	6768	6741
Tmin,Tmax	0.868,0.921	0.751,1.000
Tmin'	0.480	

Correction method= # Reported T Limits: Tmin=0.751 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.996 Theta(max)= 76.050

R(reflections)= 0.0286(6293) wR2(reflections)= 0.0773(6741)

S = 1.077 Npar= 459

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 Cl1A ..O19A . 2.85 Ang.
1/2-x,1-y,-1/2+z = 2_564 Check

Author Response: The identifed short contact has appropriate geometry for a halogen bond.

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C14 H12 Cl2 Cu N4 O2, H2 O
Rep.: H2 O, C14 H12 Cl2 Cu N4 O2
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.036 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
15 1 2, 3 1 15,

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.89 Why ?
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..... 0.00010 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..... 0.00020 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1A --N9A . 6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1B --N9B . 5.4 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 15 Note
Ha Hb Hc Hd He Hf Hg Hh
Hi Hj Hk Hl Hm Hn Ho
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 6 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 25 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
1 8 34, 3 1 15, 15 1 2,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 5.147 Note
Predicted wR2: Based on SigI**2 1.50 or SHELX Weight 7.18 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 9 Info

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```
  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
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  1 ALERT type 5 Informative message, check
```

Datablock: L2

```
Bond precision:   C-C = 0.0018 A           Wavelength=1.54184

Cell:             a=5.8777(1)     b=19.9383(3)        c=11.2632(1)
                  alpha=90        beta=95.338(1)      gamma=90
Temperature:      120 K
```

	Calculated	Reported
Volume	1314.23(3)	1314.23(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H10 Cl2 N4 O	C13 H10 Cl2 N4 O
Sum formula	C13 H10 Cl2 N4 O	C13 H10 Cl2 N4 O
Mr	309.15	309.15
Dx,g cm-3	1.562	1.562
Z	4	4
Mu (mm-1)	4.459	4.459
F000	632.0	632.0
F000'	636.45	
h,k,lmax	7,24,13	7,24,13
Nref	2611	2558
Tmin,Tmax	0.502,0.762	0.410,1.000
Tmin'	0.194	

```
Correction method= # Reported T Limits: Tmin=0.410 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.980           Theta(max)= 72.689

R(reflections)= 0.0274( 2406)                    wR2(reflections)=
                                                 0.0748( 2558)
S = 1.045                  Npar= 190
```

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

```
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           orangish
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         16 Report
               7  0  0,    7  1  0,  -7  2  1,    6  0  2,    6  1  2,  -7  2  2,
               5 10  2,    5 12  2,   6  0  4,    6  6  4,  -1  7  4,   6  7  4,
               6  1  5,    6  6  5,  -4 10  5,    5  7  7,
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         3 Note
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............   0.00010 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters         1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        37 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         1 Note
              -1  7  4,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........     3.451 Note
            Predicted wR2: Based on SigI**2  2.17 or SHELX Weight  7.15 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        13 Info
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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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

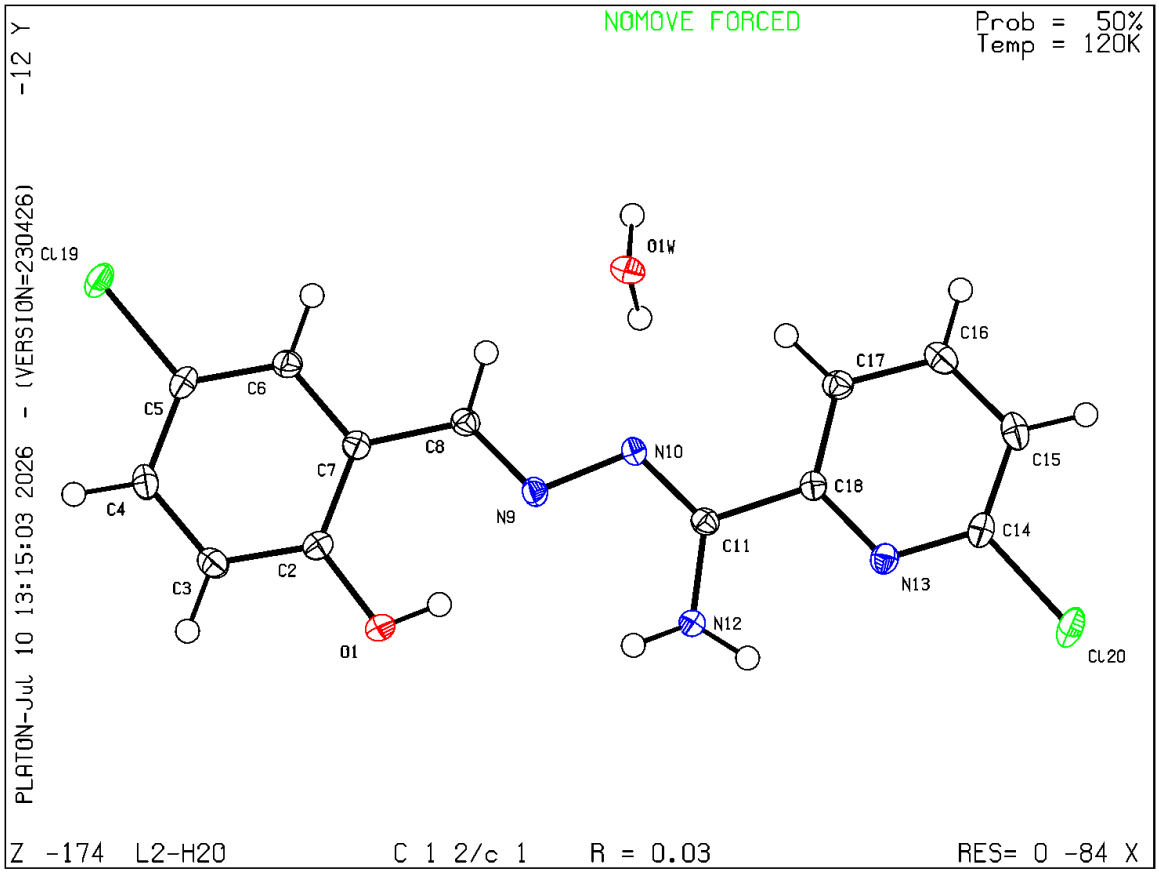
PLATON version of 23/04/2026; check.def file version of 30/03/2026

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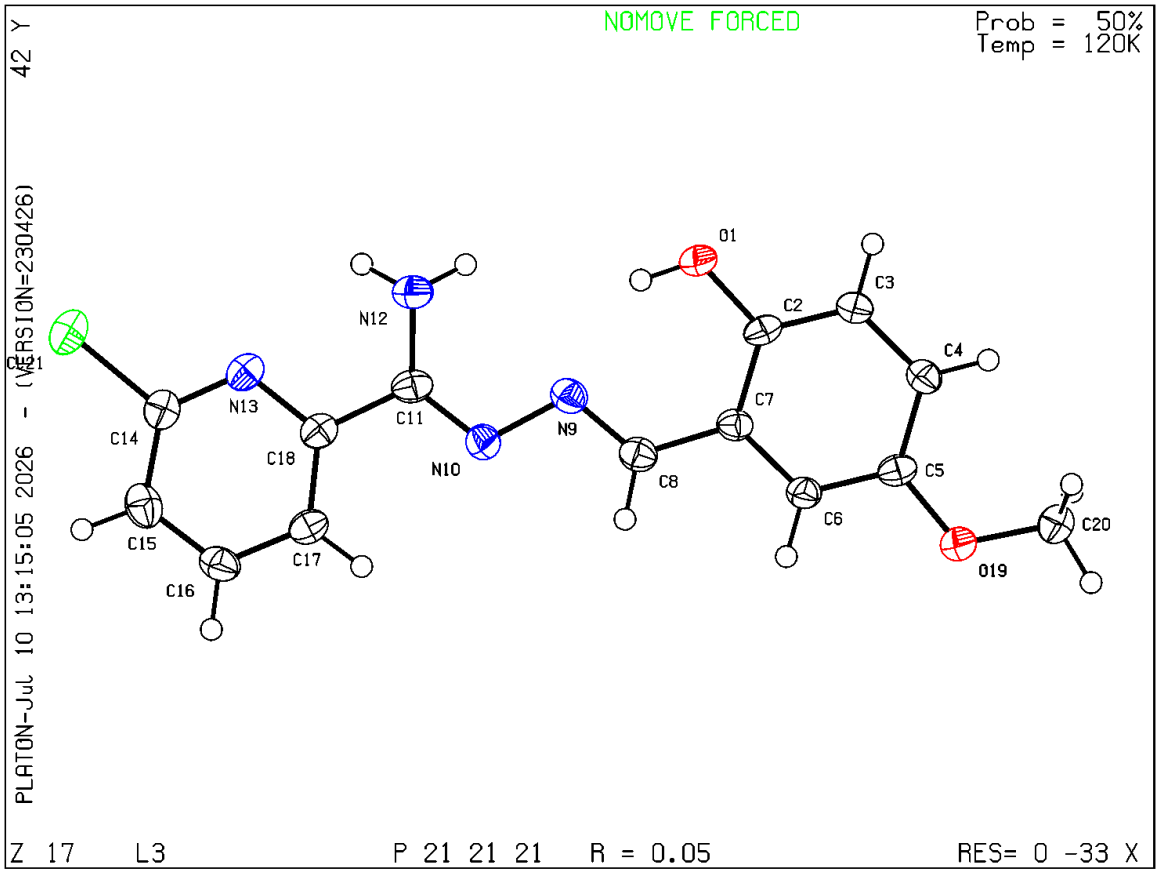
duplicate check

No duplication found

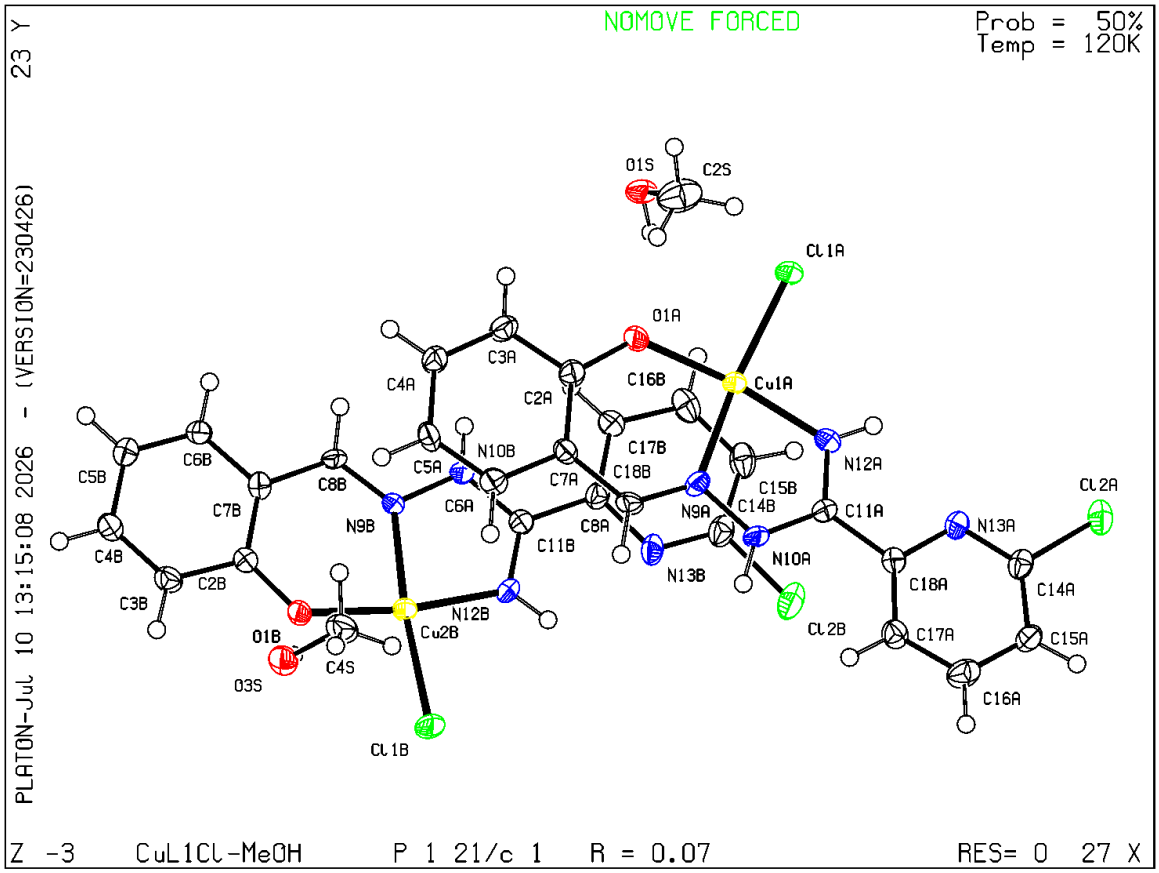
Datablock L2-H2O - ellipsoid plot



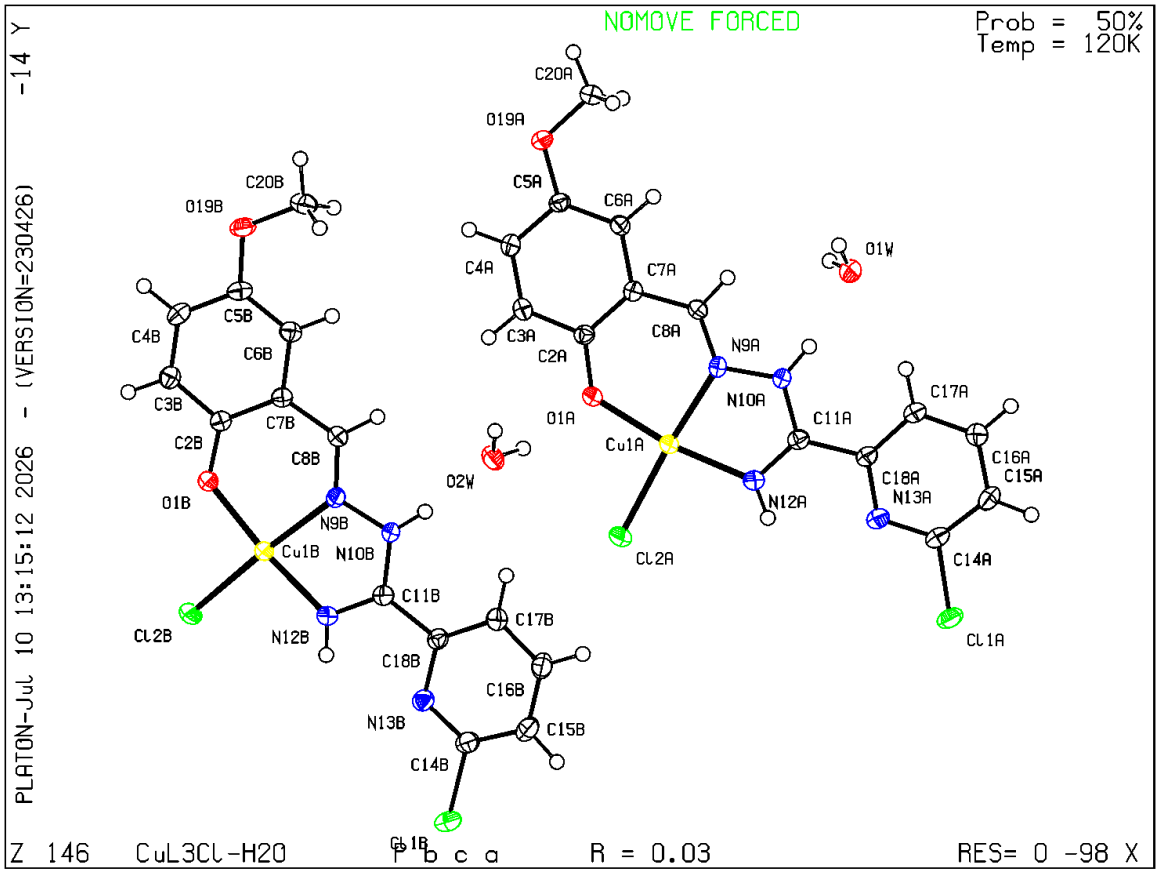
Datablock L3 - ellipsoid plot



Datablock CuL1Cl-MeOH - ellipsoid plot



Datablock CuL3Cl-H2O - ellipsoid plot



Datablock L2 - ellipsoid plot

