Supplementary data for article:

Čobeljić, B.; Pevec, A.; Turel, I.; Swart, M.; Mitić, D.; Milenković, M.; Marković, I.; Jovanović, M.; Sladić, D.; Jeremić, M.; et al. Synthesis, Characterization, DFT Calculations and Biological Activity of Derivatives of 3-Acetylpyridine and the Zinc(II) Complex with the Condensation Product of 3-Acetylpyridine and Semicarbazide. *Inorganica Chimica Acta* **2013**, *404*, 5–12. https://doi.org/10.1016/j.ica.2013.04.017

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=7.4381(1) b=11.6257(2) c=23.9731(5)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	2073.03(6)	2073.03(6)
Space group	P b c n	Pbcn
Hall group	-P 2n 2ab	?
Moiety formula	C16 H20 Cl2 N8 O2 Zn	?
Sum formula	C16 H20 Cl2 N8 O2 Zn	C16 H20 Cl2 N8 O2 Zn
Mr	492.69	492.67
Dx,g cm-3	1.579	1.579
Z	4	4
Mu (mm-1)	1.473	1.473
F000	1008.0	1008.0
F000'	1010.55	
h,k,lmax	9,15,31	9,15,31
Nref	2380	2378
Tmin,Tmax	0.795,0.863	0.757,0.867
Tmin'	0.745	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 27.480

R(reflections)= 0.0315(1827) wR2(reflections)= 0.0840(2378)

S = 1.053 Npar= 142

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

PLAT230_ALERT_2_C Hirshfeld Test Diff for O1 -- C8 .. 5.1 su

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	5
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF	?
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature	293 K
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	3

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2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 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*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

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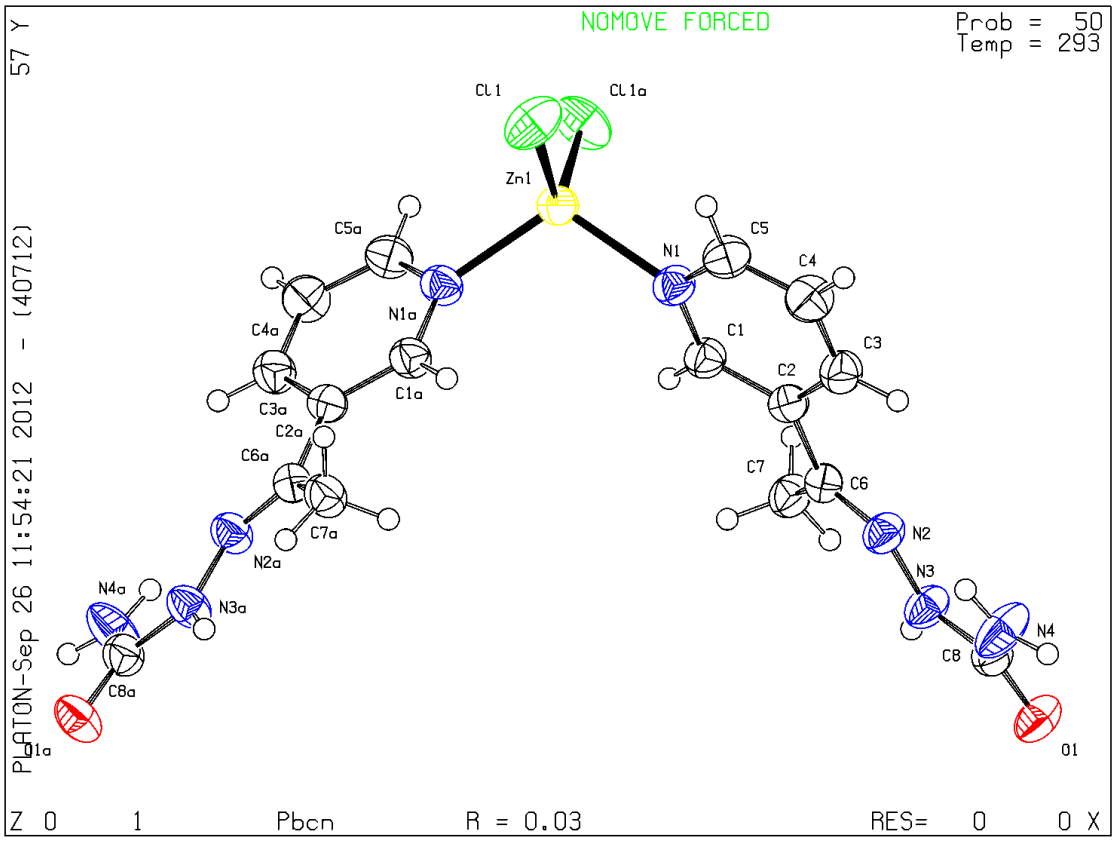
PLATON version of 04/07/2012; check.def file version of 28/06/2012

Datablock 1 - ellipsoid plot



checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: HL1

```
Bond precision:  C-C = 0.0040 A          Wavelength=0.71073

Cell:          a=6.6772(3)        b=8.9768(3)      c=11.0700(5)
               alpha=113.504(2)   beta=94.574(3)   gamma=100.428(3)
Temperature:   293 K
```

	Calculated	Reported
Volume	589.88(4)	589.88(4)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C8 H11 N4 O, Cl, 2(H2 O)	?
Sum formula	C8 H15 Cl N4 O3	C8 H15 Cl N4 O3
Mr	250.69	250.69
Dx,g cm-3	1.411	1.411
Z	2	2
Mu (mm-1)	0.324	0.324
F000	264.0	264.0
F000’	264.40	
h,k,lmax	8,11,14	8,11,14
Nref	2722	2638
Tmin,Tmax	0.981,0.984	0.938,0.984
Tmin’	0.937	

```
Correction method= MULTI-SCAN

Data completeness= 0.969          Theta(max)= 27.500

R(reflections)= 0.0571( 2190)     wR2(reflections)= 0.1594( 2638)

S = 1.178                 Npar= 170
```

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 Low 0.970

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	13
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF	?
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature	293 K
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	8

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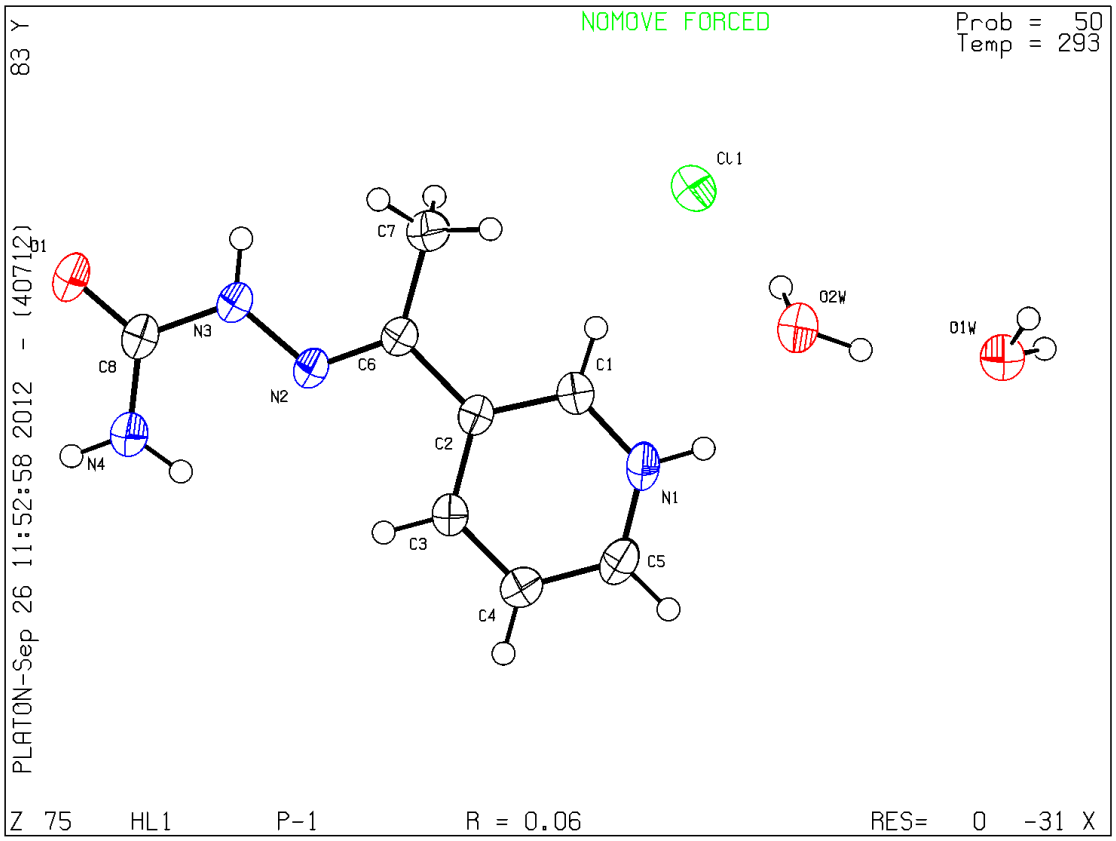
PLATON version of 04/07/2012; check.def file version of 28/06/2012

Datablock HL1 - ellipsoid plot



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: HL3

Bond precision: C-C = 0.0024 A Wavelength=0.71073

Cell: a=4.7804(2) b=9.9478(3) c=26.2508(10)
alpha=90 beta=93.338(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1246.23(8)	1246.22(8)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	C10 H14 N3 O2, Cl, H2 O	?
Sum formula	C10 H16 Cl N3 O3	C10 H16 Cl N3 O3
Mr	261.71	261.71
Dx,g cm-3	1.395	1.395
Z	4	4
Mu (mm-1)	0.308	0.308
F000	552.0	552.0
F000’	552.82	
h,k,lmax	6,12,34	6,12,34
Nref	2855	2853
Tmin,Tmax	0.964,0.970	0.861,0.970
Tmin’	0.857	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 27.480

R(reflections)= 0.0381(2237) wR2(reflections)= 0.1092(2853)

S = 1.042 Npar= 168

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 G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF	?
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature	293 K

PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 4

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Datablock HL3 - ellipsoid plot