Supplementary data for article :

Pavic, A.; Glišić, B. Đ.; Vojnovic, S.; Warżajtis, B.; Savić, N. D.; Antić, M.; Radenković, S.; Janjić, G. V.; Nikodinovic-Runic, J.; Rychlewska, U.; et al. Mononuclear Gold(III) Complexes with Phenanthroline Ligands as Efficient Inhibitors of Angiogenesis: A Comparative Study with Auranofin and Sunitinib. *Journal of Inorganic Biochemistry* **2017**, *174*, 156–168. https://doi.org/10.1016/j.jinorgbio.2017.06.009

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_7phen, 4_7phen

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_7phen

```
Bond precision:    C-C = 0.0057 A            Wavelength=0.71073

Cell:            a=12.1848(3)     b=14.1996(3)        c=7.7110(2)
                 alpha=90         beta=95.833(2)      gamma=90
Temperature:     295 K

                 Calculated               Reported
Volume           1327.24(6)               1327.24(6)
Space group      P 21/c                   P 21/c
Hall group       -P 2ybc                  -P 2ybc
Moiety formula   C12 H8 Au Cl3 N2         C12 H8 Au Cl3 N2
Sum formula      C12 H8 Au Cl3 N2         C12 H8 Au Cl3 N2
Mr               483.52                   483.52
Dx,g cm-3        2.420                    2.420
Z                4                        4
Mu (mm-1)        11.668                   11.668
F000             896.0                    896.0
F000'            890.47
h,k,lmax         14,16,9                  14,16,9
Nref             2345                     2336
Tmin,Tmax        0.502,0.705              0.093,0.780
Tmin'            0.121

Correction method= # Reported T Limits: Tmin=0.093 Tmax=0.780
AbsCorr = ANALYTICAL

Data completeness= 0.996           Theta(max)= 25.021

R(reflections)= 0.0190( 2126)      wR2(reflections)= 0.0437( 2336)

S = 1.077                   Npar= 163
```

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.

Datablock: 4_7phen

Bond precision: C-C = 0.0144 A   Wavelength=0.71073

Cell: a=7.8420(12)   b=8.8631(14)   c=10.7500(5)
               alpha=78.707(8)   beta=87.300(8)   gamma=66.988(15)
Temperature: 295 K

                   Calculated   Reported
Volume   674.04(17)   674.04(17)
Space group   P -1   P -1
Hall group   -P 1   -P 1
Moiety formula C12 H8 Au Cl3 N2   C12 H8 Au Cl3 N2
Sum formula   C12 H8 Au Cl3 N2   C12 H8 Au Cl3 N2
Mr   483.52   483.52
Dx,g cm-3   2.382   2.382
Z   2   2
Mu (mm-1)   11.488   11.488
F000   448.0   448.0
F000'   445.23
h,k,lmax   9,10,12   9,10,12
Nref   2404   4091
Tmin,Tmax   0.507,0.708   0.903,1.000
Tmin'   0.125

Correction method= # Reported T Limits: Tmin=0.903 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.702   Theta(max)= 25.061

```
R(reflections)= 0.0362( 3247)      wR2(reflections)= 0.0825( 4091)


S = 0.928                  Npar= 164
```

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**
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.01442 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min)   7 Note
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.596   10 Report

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⚪ **Alert level G**
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =   3 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..   ! Info
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still   53 % Note
PLAT931_ALERT_5_G Found Twin Law (1 1 0)[   ] Estimated BASF   0.51 Check

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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
   3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
   4 **ALERT level G** = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 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
   2 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* 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 26/02/2017; check.def file version of 21/02/2017

NOMOVE FORCED

Prob = 50
Temp = 295

-25 Y

PLATON-Mar 23 11:24:15 2017 - (70316)

Z 33   1_7phen   P 21/c   R = 0.02   RES= 0   -8 X

NOMOVE FORCED

Prob = 50
Temp = 295

61 Y

CL2

CL1

Au1

CL3

N7

C12

C8

C9

C10

C13

C14

C11

C5

C6

N4

C3

C2

C1

PLATON-Mar 23 11:24:16 2017 - (70316)

Z 132   4_7phen   P -1   R = 0.04   RES=   0   -98 X