No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: moc221

```
Bond precision:      C-C = 0.0036 A            Wavelength=0.71073
Cell:        a=7.4731(4)      b=11.7049(4)     c=17.6092(8)
             alpha=97.285(4) beta=96.617(4)  gamma=102.781(4)
Temperature
:            150 K

                   Calculated                     Reported
Volume             1473.58(12)                    1473.58(12)
Space group        P -1                           P -1
Hall group         -P 1                           -P 1
Moiety formula     C26 H22 Ag N6 O8, F6 P         C26 H22 Ag N6 O8, F6 P
Sum formula        C26 H22 Ag F6 N6 O8 P          C26 H22 Ag F6 N6 O8 P
Mr                 799.34                         799.33
Dx,g cm-3          1.801                          1.801
Z                  2                              2
Mu (mm-1)          0.837                          0.837
F000               800.0                          800.0
F000'              798.91
h,k,lmax           9,15,22                        9,15,22
Nref               6764                           6475
Tmin,Tmax          0.904,0.920                    0.841,1.000
Tmin'              0.811
Correction method= # Reported T Limits: Tmin=0.841
Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.957        Theta(max)= 27.483
R(reflections)= 0.0370( 5109)       wR2(reflections)=
                                    0.0854( 6475)
S = 1.027             Npar= 456
```

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

PLAT413_ALERT_2_B Short Inter XH3 .. XHn   H16E   ..H16E   .   1.97 Ang.
                                             1-x,2-y,1-z =   2_676 Check

Alert level C

PLAT220_ALERT_2_C NonSolvent   Resd 1 C   Ueq(max)/Ueq(min) Range   3.2 Ratio
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).   5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   9 Report

Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.004 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   1 Report
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of   P1C Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)   86% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact F7CA   ..C17A   .   2.85 Ang.
                                             x,y,z =   1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O14A   ..C6A   .   2.95 Ang.
                                             -x,1-y,1-z =   2_566 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   12 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   275 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File   1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   1.7 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.   3 Info

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.
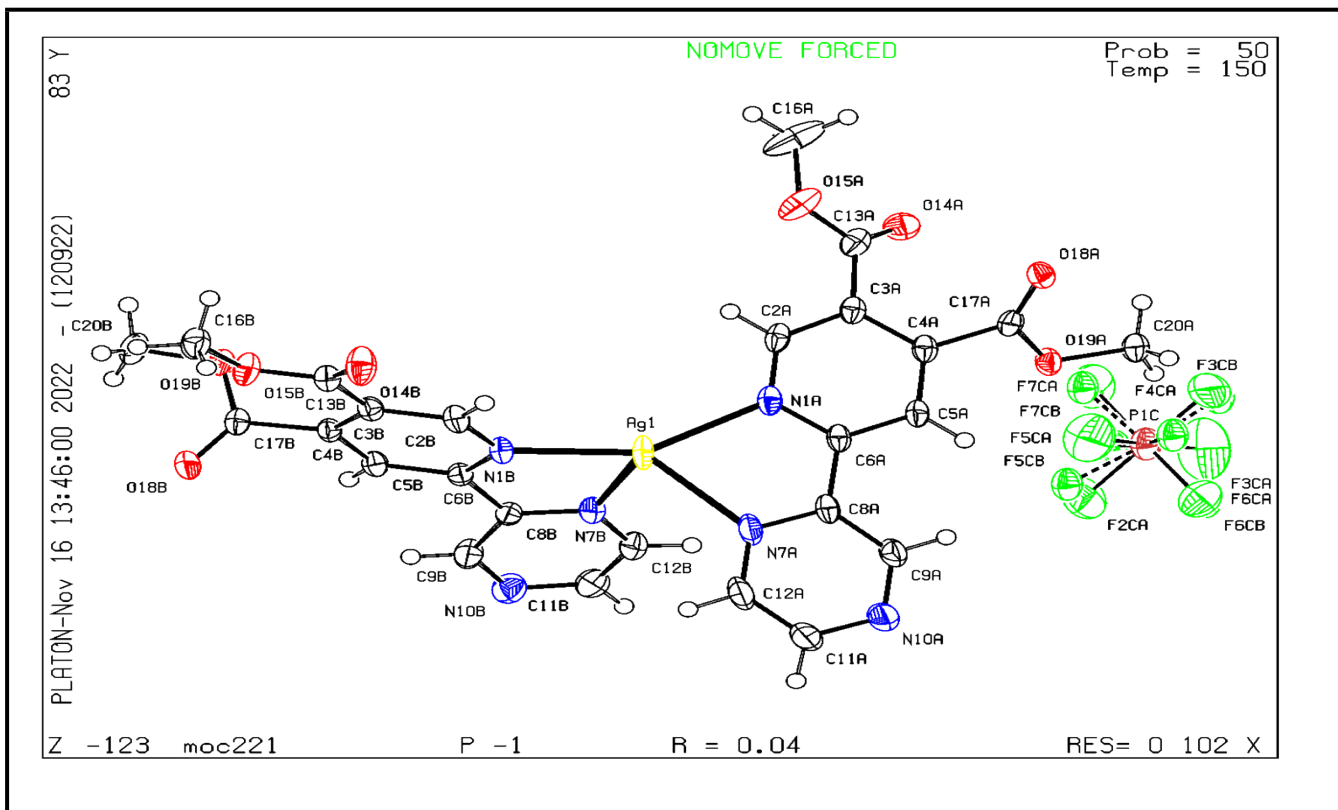
Publication of your CIF in IUCr journals

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 12/09/2022; check.def file version of 09/08/2022

Datablock moc221 - ellipsoid plot