checkCIF/PLATON report

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

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: Ag22-CBP

```
Bond precision:   C-C = 0.0138 A          Wavelength=1.54184

Cell:             a=31.2047(9)    b=14.4204(5)        c=30.1096(13)
                  alpha=90        beta=101.376(4)     gamma=90
Temperature:      100 K

                 Calculated                Reported
Volume           13282.7(9)                13282.7(8)
Space group      C 2/c                     C 1 2/c 1
Hall group       -C 2yc                    -C 2yc
Moiety formula   C55 H28 Ag11 F21 N4 O19   C55 H28 Ag11 F21 N4 O19
Sum formula      C55 H28 Ag11 F21 N4 O19   C55 H28 Ag11 F21 N4 O19
Mr               2634.39                   2634.38
Dx,g cm-3        2.635                     2.635
Z                8                         8
Mu (mm-1)        26.626                    26.627
F000             9952.0                    9952.0
F000'            9999.14
h,k,lmax         37,17,35                  37,17,35
Nref             11741                     9369
Tmin,Tmax        0.046,0.264               0.290,1.000
Tmin'            0.007

Correction method= # Reported T Limits: Tmin=0.290 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.798           Theta(max)= 66.592

R(reflections)= 0.0487( 7046)                wR2(reflections)=
                                             0.1238( 9369)
S = 1.010                 Npar= 969
```

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

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
           a literature citation. This should be contained in the
           _exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
PLAT018_ALERT_1_C _diffrn_measured_fraction_theta_max .NE. *_full          ! Check
PLAT213_ALERT_2_C Atom Ag1             has ADP max/min Ratio .....       3.2 prolat
PLAT213_ALERT_2_C Atom Ag2             has ADP max/min Ratio .....       3.7 prolat
PLAT213_ALERT_2_C Atom C1AA            has ADP max/min Ratio .....       3.6 prolat
PLAT213_ALERT_2_C Atom C25             has ADP max/min Ratio .....       3.5 prolat
PLAT213_ALERT_2_C Atom C95             has ADP max/min Ratio .....       3.1 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  F   Ueq(max)/Ueq(min) Range       3.5 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range       3.1 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       Ag1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O14 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       O18 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Ag3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      C1BA Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C20 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C51 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.01379 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C51      - C52      .      1.41 Ang.
```

Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         4 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         3 Info
PLAT012_ALERT_1_G N.O.K.   _shelx_res_checksum Found in CIF ......    Please Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records         2 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C1AA Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C24 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C26 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C28 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C30 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C52 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C67 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        1% Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C20 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C40 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for       C49 Check
PLAT343_ALERT_2_G Unusual          Angle Range in Main Residue for       C50 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         3 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...     17.80 Deg.
              AG2  -N2   -AG2A    3_545   1_555   3_545 ......     #  391 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...      2067 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       3.1 Low
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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
  20 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  23 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  30 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_ABSTY02_Ag22-CBP
;
PROBLEM: An _exptl_absorpt_correction_type has been given without
RESPONSE: ...
;
_vrf_PLAT018_Ag22-CBP
;
PROBLEM: _diffrn_measured_fraction_theta_max .NE. *_full           ! Check
RESPONSE: ...
;
_vrf_PLAT213_Ag22-CBP
;
PROBLEM: Atom Ag1             has ADP max/min Ratio .....        3.2 prolat
RESPONSE: ...
;
_vrf_PLAT220_Ag22-CBP
;
PROBLEM: NonSolvent   Resd 1  F   Ueq(max)/Ueq(min) Range        3.5 Ratio
RESPONSE: ...
;
_vrf_PLAT241_Ag22-CBP
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of        Ag1 Check
RESPONSE: ...
;
_vrf_PLAT242_Ag22-CBP
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of        Ag3 Check
RESPONSE: ...
;
_vrf_PLAT342_Ag22-CBP
;
PROBLEM: Low Bond Precision on  C-C Bonds ...............    0.01379 Ang.
RESPONSE: ...
;
_vrf_PLAT362_Ag22-CBP
;
```

```
PROBLEM: Short  C(sp3)-C(sp2) Bond  C51      - C52      .       1.41 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

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 13/07/2021; check.def file version of 13/07/2021

Datablock Ag22-CBP - ellipsoid plot