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: Ag16-CBP

Bond precision: C-C = 0.0259 A Wavelength=1.54184

Cell: a=12.5661(6) b=15.2008(6) c=17.6631(7)
alpha=84.290(3) beta=83.029(4) gamma=67.249(4)
Temperature: 293 K

	Calculated	Reported
Volume	3083.3(2)	3083.3(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C27 H15 Ag8 F27 N O21 S, C6 H16 N	C27 H13 Ag8 F25.284 N O20 S, H2 O, C6 H16 N, 1.716(F1)
Sum formula	C33 H31 Ag8 F27 N2 O21 S	C33 H31 Ag8 F27 N2 O21 S
Mr	2199.62	2199.62
Dx,g cm-3	2.369	2.369
Z	2	2
Mu (mm-1)	21.648	21.648
F000	2092.0	2092.0
F000'	2103.23	
h,k,lmax	15,18,21	14,17,21
Nref	11040	10641
Tmin,Tmax	0.097,0.339	0.033,1.000
Tmin'	0.016	

Correction method= # Reported T Limits: Tmin=0.033 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.964 Theta(max)= 67.142

R(reflections)= 0.0788(7650)

wR2(reflections)= 0.2395(10641)

S = 1.034 Npar= 649

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 A

PLAT201_ALERT_2_A Isotropic non-H Atoms in Main Residue(s) ..... 26 Report
F1 F2 F3 F4 F5 etc.

RESPONSE: F atoms are highly disordered and ANIS was not applied on F atoms.

Alert level B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.02588 Ang.

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.964 Why?
PLAT220_ALERT_2_C NonSolvent Resd 1 F Ueq(max)/Ueq(min) Range 5.8 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O6 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O13 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C3 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C9 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C20 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S9 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N3AA Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C17 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C27 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C29 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of N1 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C32 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N1 0.119 Check
PLAT314_ALERT_2_C Small Angle for H2O: Metal-O20 -H20A . 78.86 Degree
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H28C ..H29A . 1.80 Ang.
x,y,z = 1_555 Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 41 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 6 Report
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.94 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 13 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 8 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 9 Report

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PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          6 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         C8 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C12 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C14 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C16 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C18 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F1AA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F21A       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        12% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        14% Note
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for         C8 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C17      - C18      .       1.52 Ang.
PLAT410_ALERT_2_G Short Intra H...H Contact  H27B     ..H31B     .       1.62 Ang.
                                             x,y,z  =      1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact  H29B     ..H31D     .       1.56 Ang.
                                             x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H31C     ..H32C     .       1.99 Ang.
                                             x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H31D     ..H32B     .       1.99 Ang.
                                             x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H32A     ..H31B     .       2.06 Ang.
                                             x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H32C     ..H31A     .       1.81 Ang.
                                             x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H32C     ..H31B     .       1.63 Ang.
                                             x,y,z  =      1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H1B      ..H27A             2.10 Ang.
                                             x,y,z  =      1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H1B      ..H30A             1.96 Ang.
                                             x,y,z  =      1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H30A     ..H1A              2.05 Ang.
                                             x,y,z  =      1_555 Check
PLAT414_ALERT_2_G Short Intra D-H..H-X       H32A     ..H1A              2.13 Ang.
                                             x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....           8 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      76 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...     300 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........     3.9 Low
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1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
21 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
42 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
42 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
12 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

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_PLAT201_Ag16-CBP
;
PROBLEM: Isotropic non-H Atoms in Main Residue(s) .......         26 Report
RESPONSE: F atoms are highly disordered and  ANIS was not applied on F atoms.
;
_vrf_PLAT029_Ag16-CBP
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low . RESPONSE: 0.964.Why?
;
_vrf_PLAT220_Ag16-CBP
;
PROBLEM: NonSolvent   Resd 1  F   Ueq(max)/Ueq(min) Range RESPONSE: ...
;                                                              5.8 Ratio
_vrf_PLAT241_Ag16-CBP
;
PROBLEM: High   'MainMol' Ueq as Compared to Neighbors of RESPONSE: ...
;
_vrf_PLAT242_Ag16-CBP                                          06 Check
```

```
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of         S9 Check
RESPONSE: ...
;
_vrf_PLAT243_Ag16-CBP
;
PROBLEM: High   'Solvent' Ueq as Compared to Neighbors of        C27 Check
RESPONSE: ...
;
_vrf_PLAT244_Ag16-CBP
;
PROBLEM: Low    'Solvent' Ueq as Compared to Neighbors of         N1 Check
RESPONSE: ...
;
_vrf_PLAT260_Ag16-CBP
;
PROBLEM: Large Average Ueq of Residue Including        N1      0.119 Check
RESPONSE: ...
;
_vrf_PLAT314_Ag16-CBP
;
PROBLEM: Small Angle for H2O: Metal-O20      -H20A      .      78.86 Degree
RESPONSE: ...
;
_vrf_PLAT412_Ag16-CBP
;
PROBLEM: Short Intra XH3 .. XHn     H28C     ..H29A     .       1.80 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

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

Datablock Ag16-CBP - ellipsoid plot