checkCIF/PLATON report

Structure factors have been supplied for datablock(s) JA2009_148_0m

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: JA2009_148_0m

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

Cell:           a=6.0975(2)        b=8.7626(4)        c=14.6204(6)
                alpha=95.010(2)    beta=100.127(1)    gamma=90.578(2)
Temperature:    293 K

                 Calculated                 Reported
Volume           765.80(5)                  765.80(5)
Space group      P -1                       P -1
Hall group       -P 1                       -P 1
Moiety formula   C2 Ag N2 S2, C12 H10 N O   ?
Sum formula      C14 H10 Ag N3 O S2         C14 H10 Ag N3 O S2
Mr               408.24                     408.24
Dx,g cm-3        1.770                      1.770
Z                2                          2
Mu (mm-1)        1.589                      1.589
F000             404.0                      404.0
F000'            402.80
h,k,lmax         9,13,22                    9,13,22
Nref             5865                       2483
Tmin,Tmax        0.651,0.751                0.795,1.000
Tmin'            0.484

Correction method= # Reported T Limits: Tmin=0.795 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.423           Theta(max)= 33.169

R(reflections)= 0.0174( 2415)                wR2(reflections)=
                                             0.0450( 2483)
S = 1.078                  Npar= 190
```

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

```
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L=    0.600       1687 Report
```

Alert level C

```
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          5 Note
```

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for    S1       --C1       .        7.7 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    S2       --C2       .        7.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1      --S1       .       11.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1      --S2       .       19.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1      --S1_c     .       25.9 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2       ..C7       .       2.92 Ang.
                                                   1+x,y,z  =      1_655 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.13 Ratio
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       1695 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          9 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   2 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_PLAT911_JA2009_148_0m
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600       1687 Report
RESPONSE: ...
;
_vrf_PLAT913_JA2009_148_0m
;
```

```
PROBLEM: Missing # of Very Strong Reflections in FCF ....          5 Note
RESPONSE: ...
;
# end Validation Reply Form
```

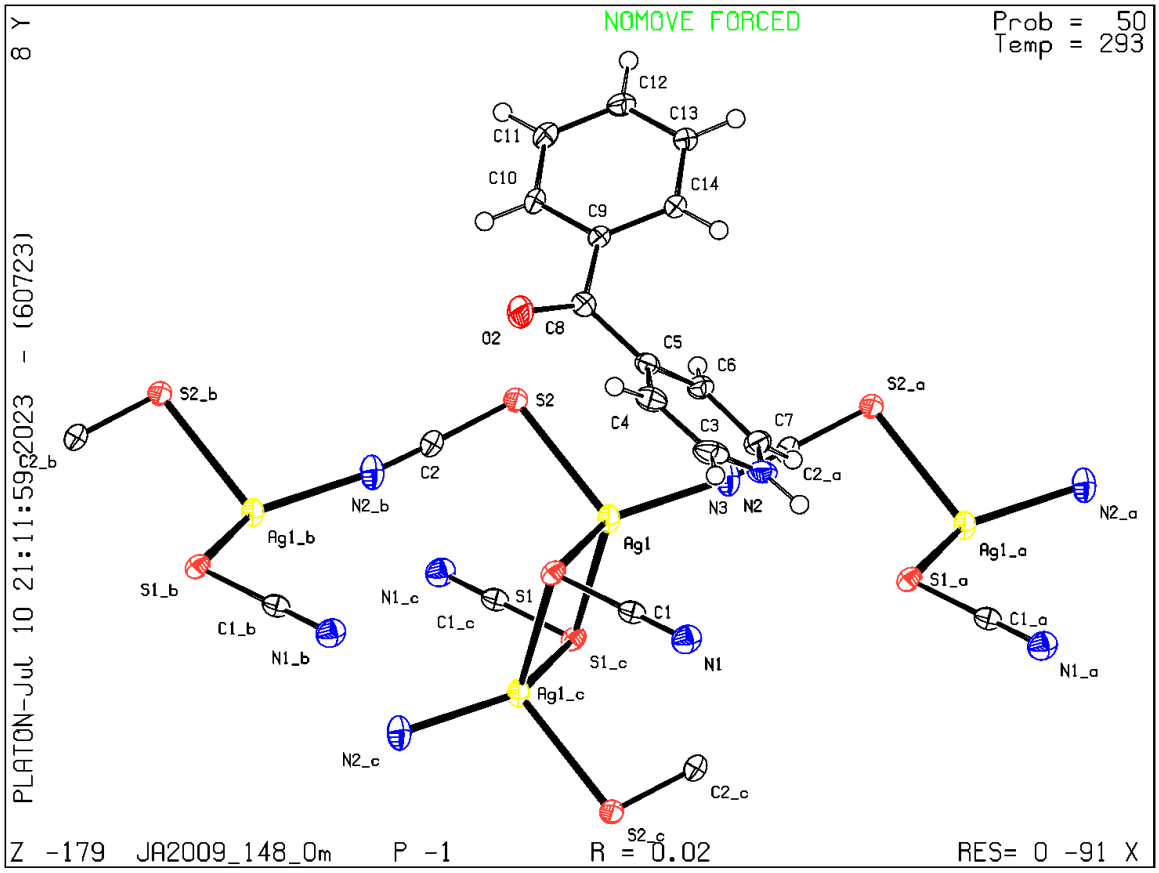
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 06/07/2023; check.def file version of 30/06/2023

Datablock JA2009_148_0m - ellipsoid plot