checkCIF/PLATON report

Structure factors have been supplied for datablock(s) agada, xsc1678_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: xsc1678_0m

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Bond precision:  C-C = 0.0129 A          Wavelength=0.71073

Cell:           a=19.2289(7)    b=18.6472(6)        c=23.2634(8)
                alpha=90        beta=112.739(1)     gamma=90
Temperature:    273 K

                Calculated                Reported
Volume          7693.1(5)                 7693.1(5)
Space group     P 21/n                    P 1 21/n 1
Hall group      -P 2yn                    -P 2yn
Moiety formula  C34 H38 Ag N10, C F3 O3 S C34 H38 Ag N10, C F3 O3 S
Sum formula     C35 H38 Ag F3 N10 O3 S    C35 H38 Ag F3 N10 O3 S
Mr              843.68                    843.68
Dx,g cm-3       1.457                     1.457
Z               8                         8
Mu (mm-1)       0.641                     0.641
F000            3456.0                    3456.0
F000'           3451.20
h,k,lmax        22,22,27                  22,20,27
Nref            13575                     12764
Tmin,Tmax       0.926,0.950               0.666,0.745
Tmin'           0.908

Correction method= # Reported T Limits: Tmin=0.666 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.940          Theta(max)= 25.018

R(reflections)= 0.0902( 9788)     wR2(reflections)= 0.2878( 12764)

S = 1.037                 Npar= 925
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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

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PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low .      0.940 Note
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min)         11 Note
PLAT972_ALERT_2_B Check Calcd Residual Density  0.15A From      O5      -3.03 eA-3
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Alert level C

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PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..................       0.29 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1   N   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 2   C   Ueq(max)/Ueq(min) Range        4.0 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 2   N   Ueq(max)/Ueq(min) Range        3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N0AA   --  C14     ..        5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N0AA   --  C15     ..        5.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N6     --  C45     ..        6.5 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N10    --  C50     ..        6.6 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    N11    --  C48     ..        5.1 s.u.
PLAT231_ALERT_4_C Hirshfeld Test (Solvent)   S1     --  O1      ..        6.1 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference N5AA   --  C31     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N4AA   --  C30     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2AA   --  C13     ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2AA   --  C14     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N2AA   --  C16     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N3AA   --  C30     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1AA   --  C12     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N1AA   --  C13     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N9     --  C46     ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N9     --  C47     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N9     --  C51     ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N10    --  C48     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N11    --  C49     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N11    --  C51     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N12    --  C65     ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N12    --  C66     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N14    --  C67     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference S1     --  O3      ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference S1     --  C69     ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F4     --  C70     ..       0.20 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      N5AA Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      N4AA Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      N3AA Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      N0AA Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C12 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C16 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        N9 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       N10 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       N11 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C63 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C64 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C66 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C67 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C11 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       C31 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C46 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C47 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C49 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C50 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C62 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C65 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        S1 Check
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PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0129 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H46B   ..  H51B    ..       1.93 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact  H48A   ..  H49B    ..       1.92 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         37 Ang3
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.391 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.595        688 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          2 Check
PLAT971_ALERT_2_C Check Calcd Residual Density  1.20A From      O6       2.09 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  0.16A From      S2       1.91 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  1.38A From     C46       1.87 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  1.04A From      O6       1.85 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  1.32A From     C50       1.73 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  1.31A From     C49       1.70 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  0.07A From     C45       1.63 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density  0.15A From      O6      -2.15 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density  0.88A From      O3      -0.43 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on    H48A      -0.33 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density           0 Note
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         16 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.17 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      31.64 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          5 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          6 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        273 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        273 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        C69 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        C70 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          7 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         34 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still          49 %
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES .........         18 Note
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ           2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ           2 Units
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  72 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  17 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  50 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
  29 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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Datablock: agada

Bond precision: C-C = 0.0024 A Wavelength=0.77490

Cell:	a=18.9803(7)	b=18.6631(7)	c=22.8795(8)
	alpha=90	beta=112.823(2)	gamma=90
Temperature:	150 K		

	Calculated	Reported
Volume	7470.1(5)	7470.1(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C40 H44 Ag N4, C F3 O3 S	C40 H44 Ag N4, C F3 O3 S
Sum formula	C41 H44 Ag F3 N4 O3 S	C41 H44 Ag F3 N4 O3 S
Mr	837.73	837.73
Dx,g cm-3	1.490	1.490
Z	8	8
Mu (mm-1)	0.814	0.814
F000	3456.0	3456.0
F000'	3457.17	
h,k,lmax	31,30,37	31,30,37
Nref	34641	34412
Tmin,Tmax		0.619,0.745
Tmin'	0.908	

Correction method= # Reported T Limits: Tmin=0.619 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 39.507

R(reflections)= 0.0397(27900) wR2(reflections)= 0.1113(34412)

S = 1.021 Npar= 955

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for C51 -- C52 .. 7.7 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C52 -- C53 .. 7.1 s.u.

Alert level C

PLAT230_ALERT_2_C Hirshfeld Test Diff for C51 -- C58 .. 6.2 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C51 -- C59 .. 6.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C55 -- C59 .. 6.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C56 -- C57 .. 5.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C71 -- C79 .. 5.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C72 -- C73 .. 5.7 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for C77 -- C78 .. 6.7 s.u.
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S2 Check
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 56 Report
PLAT971_ALERT_2_C Check Calcd Residual Density 1.41A From C52 1.89 eA-3

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PLAT971_ALERT_2_C Check Calcd Residual Density  1.33A From     C59       1.72 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  1.30A From     C58       1.61 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density          0 Note
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         3 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      5.32 Why ?
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records         2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         2 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1    --  N1      ..       5.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1    --  N3      ..       5.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag2    --  N5      ..       5.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag2    --  N8      ..       5.3 s.u.
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       C81 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of       C82 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        23 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       170 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         2 Note
PLAT933_ALERT_2_G Number of OMIT records in Embedded RES .........        57 Note
PLAT984_ALERT_1_G The  H-f'=     0.000 Deviates from the B&C-Value     0.011 Check
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```
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   4 ALERT type 3 Indicator that the structure quality may be low
   7 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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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

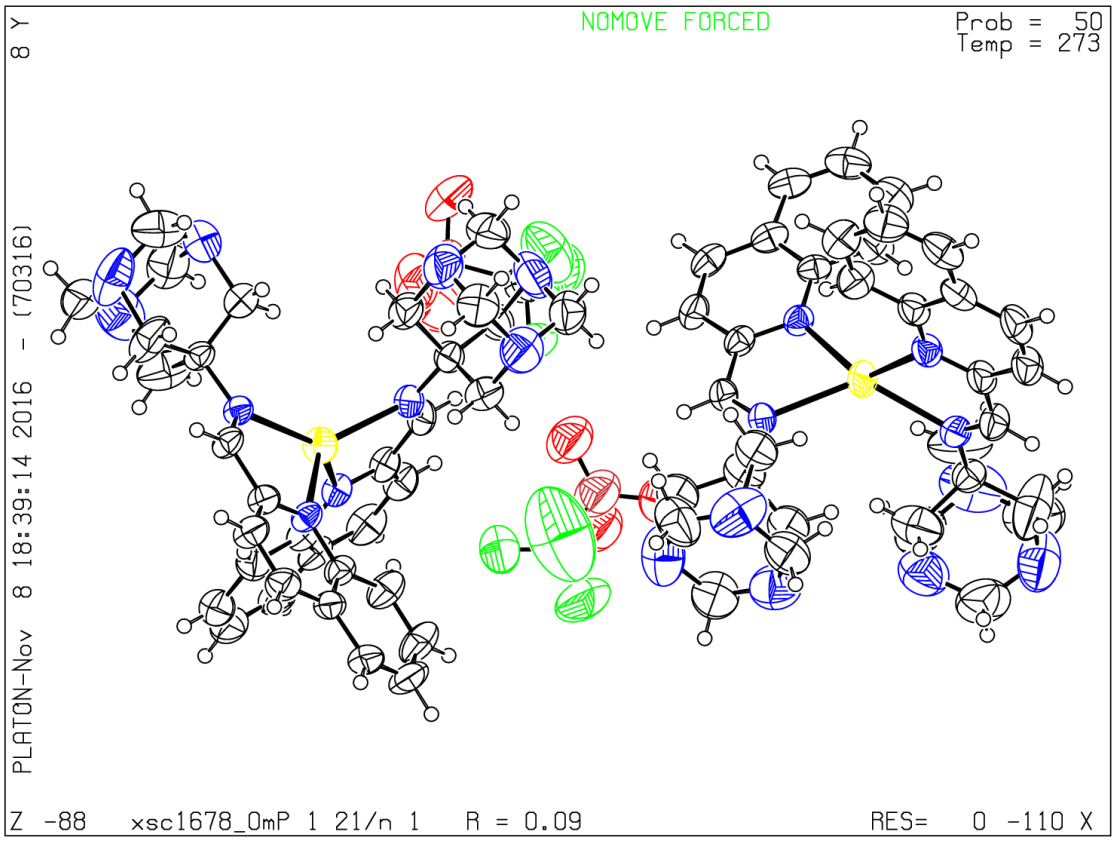
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 11/08/2016; check.def file version of 04/08/2016

Datablock xsc1678_0m - ellipsoid plot



Datablock agada - ellipsoid plot