checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compound1

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: compound1

```
Bond precision:   C-C = 0.0092 A          Wavelength=0.71073

Cell:               a=8.0211(13)      b=17.506(3)      c=25.923(4)
                    alpha=90          beta=90          gamma=90
Temperature:        298 K
```

	Calculated	Reported
Volume	3640.0(10)	3640.1(10)
Space group	I m a 2	I m a 2
Hall group	I 2 -2a	I 2 -2a
Moiety formula	C16 H27 Ag6 S4, 2(B F4) [+ solvent]	?
Sum formula	C16 H27 Ag6 B2 F8 S4 [+ solvent]	C16 H36 Ag6 B2 F8 S4
Mr	1168.46	1177.53
Dx,g cm-3	2.132	2.149
Z	4	4
Mu (mm-1)	3.441	3.442
F000	2204.0	2240.0
F000'	2185.31	
h,k,lmax	9,20,30	9,20,30
Nref	3487[1786]	2895
Tmin,Tmax		0.580,0.745
Tmin'		

```
Correction method= # Reported T Limits: Tmin=0.580 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.62/0.83        Theta(max)= 25.022
```

R(reflections)= 0.0419(1939)

wR2(reflections)= 0.1178(2895)

S = 1.080 Npar= 197

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 C7 --C9 . 10.3 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C10 --C11 . 9.0 s.u.
PLAT260_ALERT_2_B Large Average Ueq of Residue Including F1 0.311 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including F4 0.332 Check
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C2 Check
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C6 Check
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing). C12 Check
PLAT412_ALERT_2_B Short Intra XH3 .. XHn H3B ..H3B . 1.77 Ang.
3/2-x,y,z = 4_655 Check
PLAT936_ALERT_2_B The Embedded .res File Includes a DAMP Command . 5000.0 Report
PLAT987_ALERT_1_B The Flack x is >> 0 - Do a BASF/TWIN Refinement Please Check

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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
STRVA01_ALERT_4_C Flack test results are ambiguous.
From the CIF: _refine_ls_abs_structure_Flack 0.460
From the CIF: _refine_ls_abs_structure_Flack_su 0.080
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 3 Check
F1 B1 B2
PLAT213_ALERT_2_C Atom C3 has ADP max/min Ratio ..... 3.5 prolat
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag2 --S4 . 8.9 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag4 --S3 . 5.8 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C1 --C3 . 0.18 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Ag2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Ag6 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00917 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.451 Report
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= 0.595 8 Report

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Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C16 H36 Ag6 B2 F8 S4
           Atom count from the _atom_site data:  C16 H27 Ag6 B2 F8 S4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C16 H36 Ag6 B2 F8 S4
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         64.00     64.00    0.00
          H        144.00    108.00   36.00
          Ag        24.00     24.00    0.00
          B          8.00      8.00    0.00
          F         32.00     32.00    0.00
          S         16.00     16.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         24 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         12 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      23.09 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          4 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          2 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          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag3A     --S2       .        9.1 s.u.
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of         B1 Check
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of         B2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8B        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H8C        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         6% Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C2 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for         C6 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for         C7 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C12 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C1       - C2       .       1.54 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C4       - C6       .       1.54 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C7       - C8       .       1.50 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C10      - C12      .       1.51 Ang.
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H8B      ..H9B      .       2.00 Ang.
                                                    x,y,z  =      1_555 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        185 A**3
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.21 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Ag2       (I)       .       1.08 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ag4       (I)       .       1.02 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ag6       (I)       .       0.90 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         73 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        32% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         1 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage         66 %
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........       4.9 Low
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PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
  10 ALERT level B = A potentially serious problem, consider carefully
  23 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  43 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  38 ALERT type 2 Indicator that the structure model may be wrong or deficient
  11 ALERT type 3 Indicator that the structure quality may be low
  14 ALERT type 4 Improvement, methodology, query or suggestion
   4 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

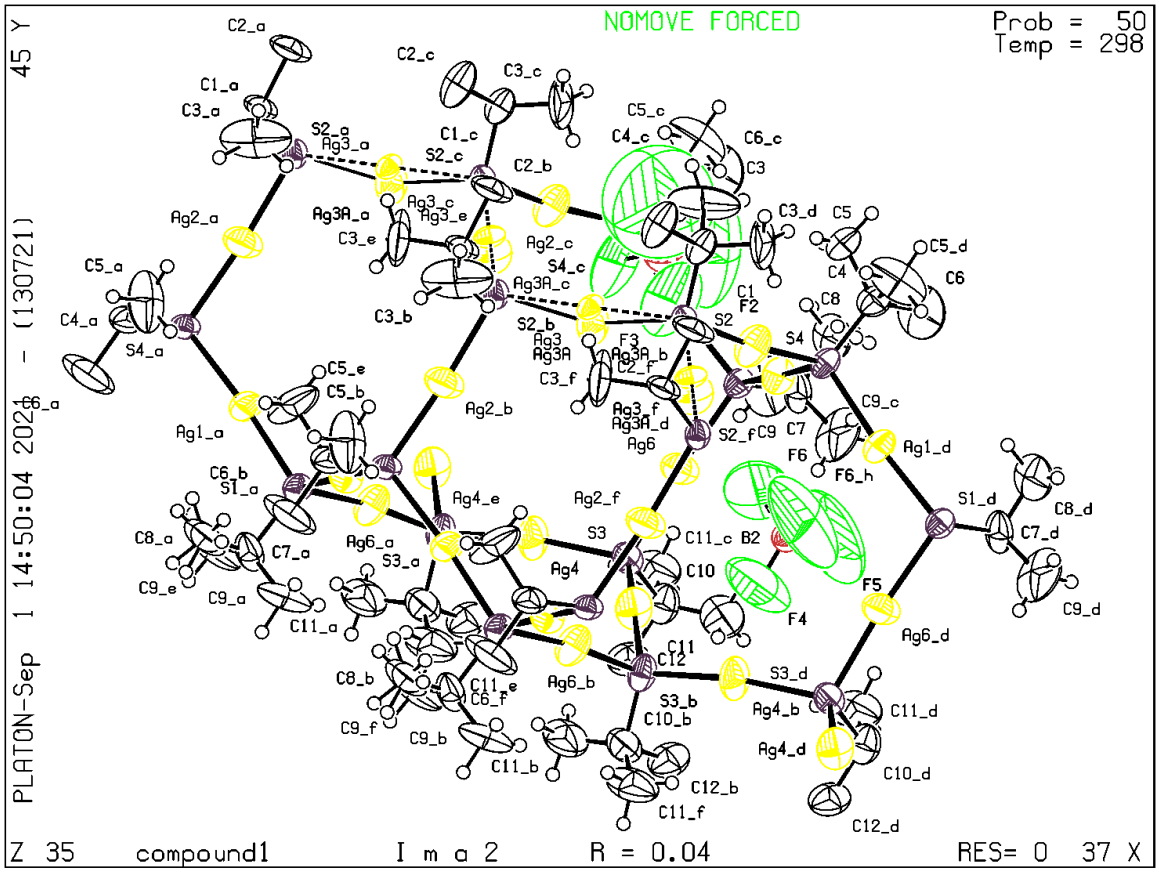
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

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

Datablock compound1 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compound2

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: compound2

Bond precision: C-C = 0.0110 A Wavelength=0.71073

Cell: a=28.993(3) b=13.3666(13) c=30.602(3)
alpha=90 beta=103.405(2) gamma=90
Temperature: 172 K

	Calculated	Reported
Volume	11536(2)	11536.4(19)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C62 H91 Ag19 F24 N3 O21 S10 [+ solvent]	?
Sum formula	C62 H91 Ag19 F24 N3 O21 S10 [+ solvent]	C62 H98 Ag19 F24 N3 O21 S10
Mr	4040.51	4047.56
Dx,g cm-3	2.326	2.330
Z	4	4
Mu (mm-1)	3.416	3.416
F000	7684.0	7712.0
F000'	7624.29	
h,k,lmax	32,14,33	32,14,33
Nref	16556	16493
Tmin,Tmax		0.005,0.018
Tmin'		

Correction method= # Reported T Limits: Tmin=0.005 Tmax=0.018
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 23.257

R(reflections)= 0.0735(14066)

wR2(reflections)= 0.2153(16493)

S = 1.056 Npar= 1322

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

```
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =    0.5556
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......          3 Report
              O8        O51       O52
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of         O9 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of        O16 Check
PLAT241_ALERT_2_B High   'MainMol' Ueq as Compared to Neighbors of        O51 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        C33 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        C37 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        C47 Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of        C49 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O6       ..O52      .       2.72 Ang.
                                                2-x,-y,1-z  =      3_756 Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).         30 Note
PLAT936_ALERT_2_B The Embedded .res File Includes a DAMP Command .     5000.0 Report
```

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
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT213_ALERT_2_C Atom F7              has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom F12             has ADP max/min Ratio .....        3.4 prolat
PLAT213_ALERT_2_C Atom C31             has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C38             has ADP max/min Ratio .....        3.4 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        4.7 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        3.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.1 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O11 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O17 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O18 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O19 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         N3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C58 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Ag6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Ag9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Ag14 Check
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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Ag16 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S7 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S8 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       S10 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C1 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       C13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C25 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C29 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C32 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C43 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C45 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C51 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C53 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C55 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C59 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C61 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Ag1      0.121 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ...........       O13 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01105 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C33      - C35      .      1.42 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C29      - C42      .      1.71 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C29      - C30      .      1.39 Ang.
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C31      - C33      .      1.33 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact  F7       ..O52      .      2.72 Ang.
                                                2-x,-y,1-z  =      3_756 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.206 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.556        32 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.54A   From O52           -1.32 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  0.66A   From O52           -0.95 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H2AC            -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H27C            -0.33 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H38B            -0.60 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H42B            -0.37 eA-3
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C62 H98 Ag19 F24 N3 O21 S10
           Atom count from the _atom_site data:  C62 H91 Ag19 F24 N3 O21 S10
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C62 H98 Ag19 F24 N3 O21 S10
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        248.00    248.00    0.00
          H        392.00    364.00   28.00
          Ag        76.00     76.00    0.00
          F         96.00     96.00    0.00
          N         12.00     12.00    0.00
          O         84.00     84.00    0.00
          S         40.00     40.00    0.00
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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         36 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        108 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of A11A     as         AG
PLAT017_ALERT_1_G Check Scattering Type Consistency of A10A     as         AG
PLAT017_ALERT_1_G Check Scattering Type Consistency of A12A     as         AG
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     273.25 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         11 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          6 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C34 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C44 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C46 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C48 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C50 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        C54 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C62 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         5% Note
PLAT303_ALERT_2_G Full Occupancy Atom H7AC      with # Connections       1.07 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for        C48 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for        C50 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F2       ..C26             2.92 Ang.
                                      3/2-x,-1/2+y,1/2-z  =      2_645 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         15 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C29      --C42             1.71 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        610 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        69% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          4 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.9 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

---

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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
81 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
7 ALERT type 4 Improvement, methodology, query or suggestion
1 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

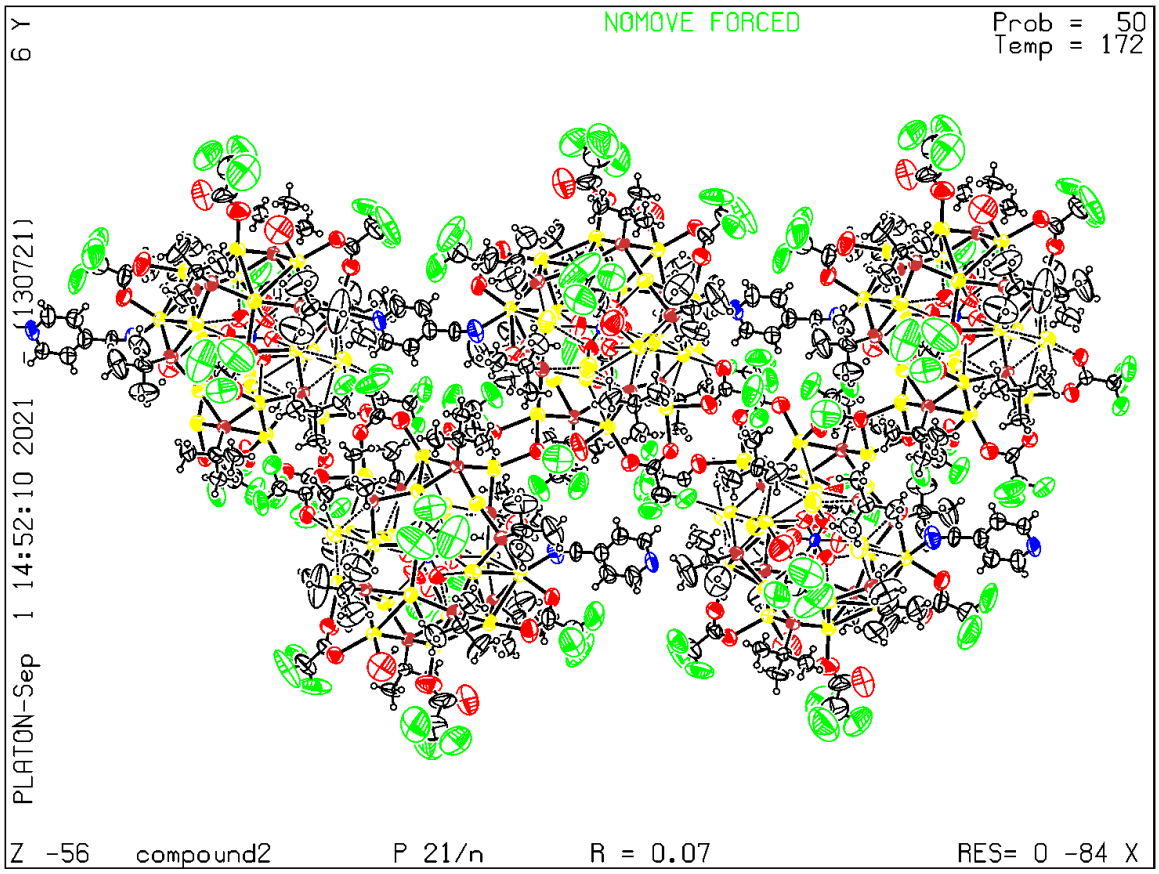
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

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

Datablock compound2 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compound3

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: compound3

Bond precision: C-C = 0.0187 A Wavelength=0.71073

Cell: a=13.5484(15) b=15.7398(17) c=16.2419(18)
alpha=118.629(2) beta=103.322(2) gamma=99.445(3)
Temperature: 173 K

	Calculated	Reported
Volume	2801.4(5)	2801.4(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C65 H102 Ag20 F24 N4 O22 S10	?
Sum formula	C65 H102 Ag20 F24 N4 O22 S10	C65 H102 Ag20 F24 N4 O19 S10
Mr	4225.51	4177.50
Dx,g cm-3	2.505	2.476
Z	1	1
Mu (mm-1)	3.690	3.686
F000	2012.0	1988.0
F000'	1996.20	
h,k,lmax	16,18,19	16,18,19
Nref	9891	9633
Tmin,Tmax		0.285,0.745
Tmin'		

Correction method= # Reported T Limits: Tmin=0.285 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.974 Theta(max)= 25.027

R(reflections)= 0.0583(9081)

wR2(reflections)= 0.1571(9633)

S = 1.087 Npar= 680

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

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 48.01 Check
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 3 Report
F5 C19 C101
PLAT213_ALERT_2_B Atom C20 has ADP max/min Ratio ..... 4.1 prolat
PLAT213_ALERT_2_B Atom C24 has ADP max/min Ratio ..... 4.6 prolat
PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 10.0 Ratio
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O6 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O11 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C23 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C101 Check

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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
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.974 Why?
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT213_ALERT_2_C Atom F4 has ADP max/min Ratio ..... 3.6 prolat
PLAT213_ALERT_2_C Atom F6 has ADP max/min Ratio ..... 3.4 prolat
PLAT213_ALERT_2_C Atom F8 has ADP max/min Ratio ..... 3.9 prolat
PLAT213_ALERT_2_C Atom C25 has ADP max/min Ratio ..... 3.7 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 F Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.1 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag1 --O5_a . 6.4 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag3 --S2_a . 5.6 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag5 --S4 . 6.4 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag8 --S5_a . 7.5 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag10 --O5 . 6.6 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ag6 --O6 . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ag9 --O11 . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ag10 --O11_a . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference A6A --O6 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O5 --O6 . 0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O5 --O11_a . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O11 --O5_a . 0.22 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O2 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O3 Check

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PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O9 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O10 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Ag9 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        C18 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C28 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        C33 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01867 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.924 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         8 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595       252 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....        11 Note
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.91A   From Ag2             1.93 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.08A   From Ag2             1.66 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.88A   From Ag1             1.64 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.06A   From Ag5             1.58 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.80A   From Ag9             1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.80A   From Ag9            -2.37 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.92A   From Ag10           -1.97 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.62A   From Ag5            -1.97 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.88A   From Ag4            -1.90 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.78A   From Ag10           -1.82 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.87A   From Ag8            -1.81 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.93A   From Ag1            -1.78 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.82A   From Ag6            -1.70 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.54A   From O5             -1.60 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.88A   From Ag2            -1.57 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.97A   From Ag3            -1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.77A   From Ag3            -1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.57A   From O5             -1.56 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.88A   From Ag4            -1.53 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H24A             -0.33 eA-3
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C65 H102 Ag20 F24 N4 O19 S10
           Atom count from the _atom_site data:  C65 H102 Ag20 F24 N4 O22 S10
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    1
          From the CIF: _chemical_formula_sum  C65 H102 Ag20 F24 N4 O19 S10
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C         65.00     65.00    0.00
          H        102.00    102.00    0.00
          Ag        20.00     20.00    0.00
          F         24.00     24.00    0.00
          N          4.00      4.00    0.00
          O         19.00     22.00   -3.00
          S         10.00     10.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         4 Note
```

```
PLAT017_ALERT_1_G Check Scattering Type Consistency of A6A      as         AG
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      34.73 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag6      --O5       .        6.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  A6A      --O5       .        5.4 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C27 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C29 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        C32 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         6% Note
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for       C101 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C28      - C29      .       1.50 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          1 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.17 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         86% Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.8 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
64 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
0 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

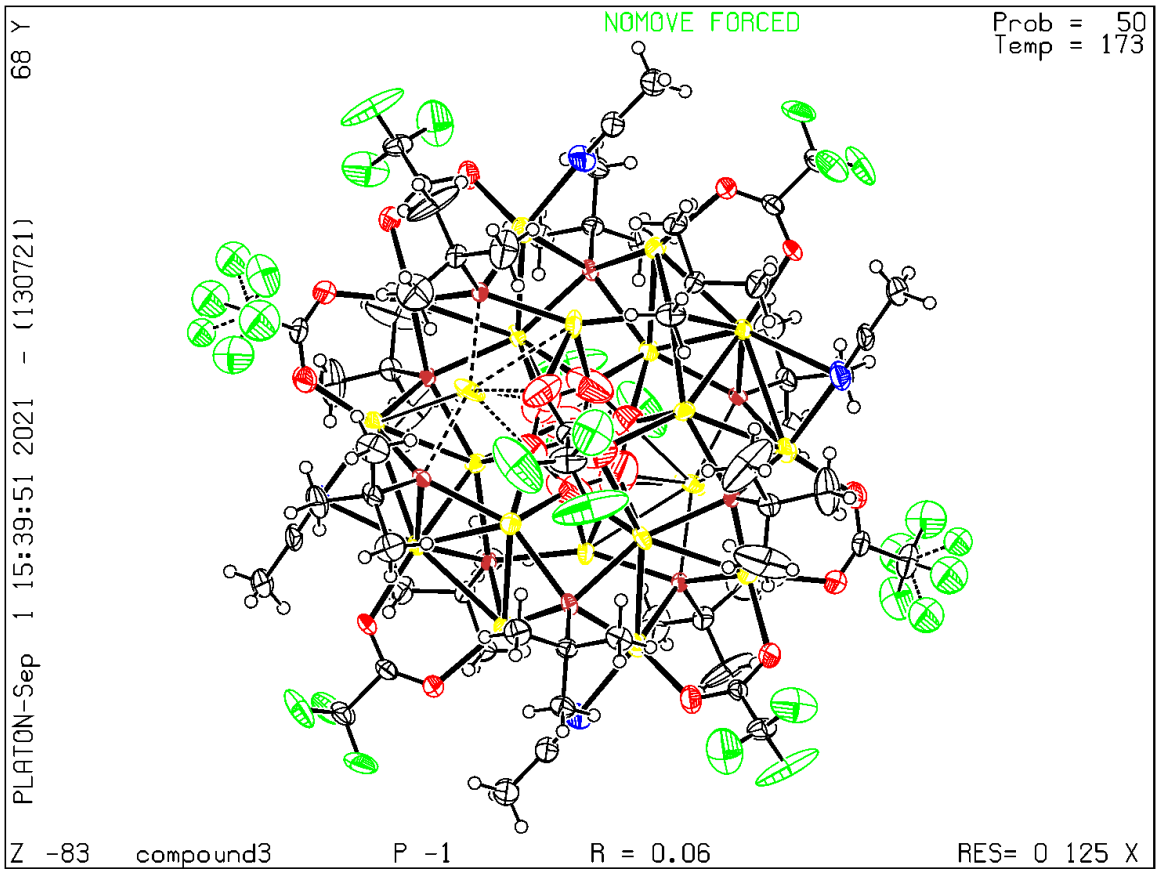
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

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

Datablock compound3 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compound4

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: compound4

```
Bond precision:   C-C = 0.0410 A          Wavelength=0.71073

Cell:           a=18.149(3)        b=18.817(3)       c=26.043(5)
                alpha=68.967(4)    beta=79.628(6)    gamma=76.198(4)
Temperature:    293 K
```

	Calculated	Reported
Volume	8018(2)	8018(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C68 H162 Ag22 O25 P9 S26 V2, C O, 2(O) [+ solvent]	?
Sum formula	C69 H162 Ag22 O28 P9 S26 V2 [+ solvent]	C73 H187 Ag22 O33 P9 S26 V2
Mr	5027.25	5180.52
Dx,g cm-3	2.082	2.146
Z	2	2
Mu (mm-1)	3.204	3.210
F000	4862.0	5040.0
F000'	4833.23	
h,k,lmax	20,20,28	20,20,28
Nref	23013	22912
Tmin,Tmax	0.636,0.725	0.596,0.740
Tmin'	0.556	

```
Correction method= # Reported T Limits: Tmin=0.596 Tmax=0.740
AbsCorr = MULTI-SCAN

Data completeness= 0.996           Theta(max)= 23.256
```

R(reflections)= 0.0704(14725)

wR2(reflections)= 0.1956(22912)

S = 0.993 Npar= 1404

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

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575
Calculated sin(theta_max)/wavelength = 0.5555

PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ..... 4 Report
S18A O25 C26 C36

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ag2 --S24 . 11.5 s.u.
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ag20 --S2 . 12.3 s.u.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C21 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C35 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of P9 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C41 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C53 Check
PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C65 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1W Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O2W Check
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.04095 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C13 - C14 . 1.26 Ang.
PLAT360_ALERT_2_B Short C(sp3)-C(sp3) Bond C15 - C16 . 1.30 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 48 Note

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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

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 4 Check
O101 C101 O1W O2W

PLAT213_ALERT_2_C Atom O24 has ADP max/min Ratio ..... 3.8 oblate
PLAT213_ALERT_2_C Atom C42 has ADP max/min Ratio ..... 3.4 prolat
PLAT213_ALERT_2_C Atom C54 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C55 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C56 has ADP max/min Ratio ..... 3.6 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 5.1 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 4.7 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 S Ueq(max)/Ueq(min) Range 5.7 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag2 --S23 . 5.5 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag5 --S20 . 6.5 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag6 --S23 . 6.0 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag6 --S24 . 6.5 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag7 --S3 . 6.7 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag9 --S8 . 5.3 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag10 --S17 . 6.0 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag11 --S10 . 6.0 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag19 --S1 . 6.8 s.u.
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag19 --S3 . 5.7 s.u.

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PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Ag21     --S20      .        5.5 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ag10     --O2       .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ag18     --O6       .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference S26      --C65      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1       --O8       .       0.19 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        S12 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        S16 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O23 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O24 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         C7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C15 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C27 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       Ag21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         V1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S19 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S20 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S23 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S24 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S25 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        S26 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         P1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         P5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         P6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         P8 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         O6 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         O8 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         O9 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O14 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O18 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O19 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O20 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O25 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C13 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        C25 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C37 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C45 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        C57 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C61 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Ag1     0.123 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) .....          O101 Check
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C1       - C2       .       1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C3       - C4       .       1.42 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C9       - C10      .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C11      - C12      .       1.35 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C17      - C18      .       1.34 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C27      - C28      .       1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C29      - C30      .       1.36 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C31      - C32      .       1.36 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C41      - C43      .       1.42 Ang.
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PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C53      - C54      .       1.41 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C53      - C56      .       1.40 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C65      - C66      .       1.38 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H7B      ..H24C     .       2.05 Ang.
                                                  -x,-y,2-z  =      2_557 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.556         55 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          6 Note
PLAT976_ALERT_2_C Check Calcd Resid. Dens.  1.02A   From O3            -0.63 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H15B            -0.34 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H35A            -0.36 eA-3
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C73 H187 Ag22 O33 P9 S26 V2
           Atom count from the _atom_site data:  C69 H162 Ag22 O28 P9 S26 V2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C73 H187 Ag22 O33 P9 S26 V2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        146.00    138.00    8.00
          H        374.00    324.00   50.00
          Ag        44.00     44.00    0.00
          O         66.00     56.00   10.00
          P         18.00     18.00    0.00
          S         52.00     52.00    0.00
          V          4.00      4.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         14 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         80 Report
PLAT017_ALERT_1_G Check Scattering Type Consistency of A14A     as         AG
PLAT017_ALERT_1_G Check Scattering Type Consistency of A15A     as         AG
PLAT017_ALERT_1_G Check Scattering Type Consistency of A18A     as         AG
PLAT017_ALERT_1_G Check Scattering Type Consistency of A22A     as         AG
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     136.52 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          4 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          1 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag14     --S21      .       19.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag15     --S14      .        5.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag18     --S15      .       10.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag22     --S26      .        6.0 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         4% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  2  )       1.26 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )       0.74 Check
PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing).       C101 Check
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PLAT315_ALERT_2_G Singly Bonded Carbon Detected (H-atoms Missing).       C102 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for        C17 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for        C33 Check
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O24            48.6 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1W      ..C102            2.14 Ang.
                                          1-x,1-y,1-z  =      2_666 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1W      ..C101            2.59 Ang.
                                          1-x,1-y,1-z  =      2_666 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure .....          ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .......          4 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #        5 Note
            O
PLAT794_ALERT_5_G Tentative Bond Valency for Ag20      (I)       .       1.14 Info
PLAT794_ALERT_5_G Tentative Bond Valency for V1        (V)       .       5.12 Info
PLAT794_ALERT_5_G Tentative Bond Valency for V2        (V)       .       5.07 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ............       375 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed         ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       32% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...        1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........       3.6 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged    Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        0 Info
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```
  0 ALERT level A = Most likely a serious problem - resolve or explain
 16 ALERT level B = A potentially serious problem, consider carefully
 86 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 48 ALERT level G = General information/check it is not something unexpected

 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
109 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
 17 ALERT type 4 Improvement, methodology, query or suggestion
  3 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

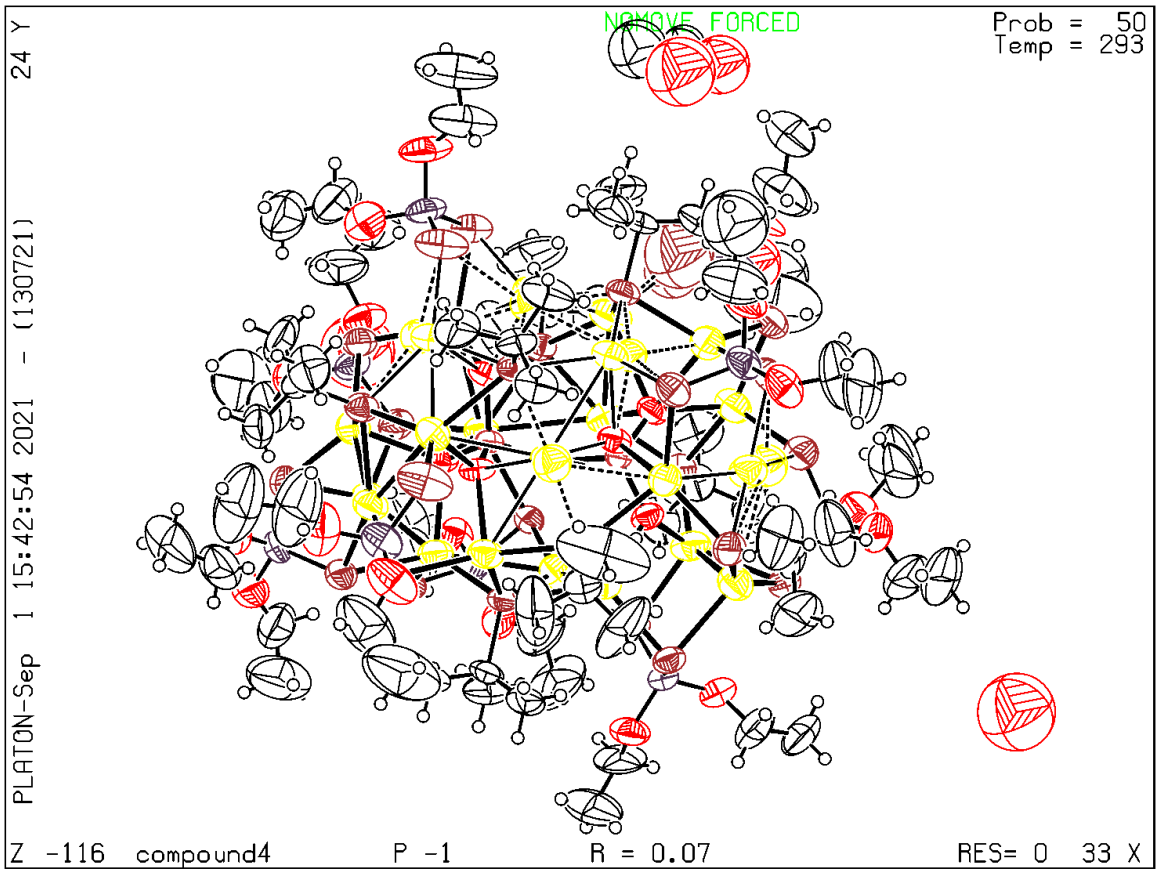
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

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

Datablock compound4 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) compound5

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: compound5

Bond precision: C-C = 0.0415 A Wavelength=0.71073

Cell: a=18.3286(5) b=18.3286(5) c=30.1460(17)
alpha=90 beta=90 gamma=120
Temperature: 298 K

	Calculated	Reported
Volume	8770.4(7)	8770.4(7)
Space group	P 63/m	P 63/m
Hall group	-P 6c	-P 6c
Moiety formula	C92 H171 Ag24.05 O21 P6 S26 W2 [+ solvent]	?
Sum formula	C92 H171 Ag24.05 O21 P6 S26 W2 [+ solvent]	C92 H210 Ag24 O21 P6 S26 W2
Mr	5594.73	5628.55
Dx,g cm-3	2.119	2.131
Z	2	2
Mu (mm-1)	4.329	4.324
F000	5350.8	5424.0
F000'	5313.30	
h,k,lmax	20,20,33	20,20,33
Nref	4227	4213
Tmin,Tmax	0.641,0.720	0.441,0.746
Tmin'	0.629	

Correction method= # Reported T Limits: Tmin=0.441 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 23.093

R(reflections)= 0.0845(3588)

wR2(reflections)= 0.2248(4213)

S = 0.958 Npar= 381

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

```
THETM01_ALERT_3_B  The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =    0.5519
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......          3 Report
             O4        C8        C12
PLAT213_ALERT_2_B Atom Ag4B            has ADP max/min Ratio .....        4.7 prolat
PLAT220_ALERT_2_B NonSolvent   Resd 1 Ag   Ueq(max)/Ueq(min) Range        9.0 Ratio
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing).        C12 Check
PLAT315_ALERT_2_B Singly Bonded Carbon Detected (H-atoms Missing).        C17 Check
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ...............    0.04154 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).         12 Note
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on      Ag1B       1.56 eA-3
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Alert level C

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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
SHFSU01_ALERT_2_C  The absolute value of parameter shift to su ratio > 0.05
           Absolute value of the parameter shift to su ratio given   0.056
           Additional refinement cycles may be required.
PLAT080_ALERT_2_C Maximum Shift/Error ............................       0.06 Why ?
PLAT213_ALERT_2_C Atom Ag3C            has ADP max/min Ratio .....        3.6 prolat
PLAT213_ALERT_2_C Atom C3B             has ADP max/min Ratio .....        3.2 oblate
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        3.1 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference W1       --O2       .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ag2B     --C6       .       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ag3B     --S1       .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference Ag3B     --S5       .       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1       --O3A      .       0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O3A      --C16      .       0.24 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         S2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S5 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C8 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.552          3 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          3 Check
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Ag1A       1.44 eA-3
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PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.77A   From O1              1.01 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.80A   From O1              0.89 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.56A   From O1              0.75 eA-3
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C92 H210 Ag24 O21 P6 S26 W2
           Atom count from the _atom_site data:  C92 H174 Ag24.05100 O21 P6 S26 W
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
          From the CIF: _cell_formula_units_Z    2
          From the CIF: _chemical_formula_sum  C92 H210 Ag24 O21 P6 S26 W2
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        184.00    184.00    0.00
          H        420.00    348.00   72.00
          Ag        48.00     48.10   -0.10
          O         42.00     42.00    0.00
          P         12.00     12.00    0.00
          S         52.00     52.00    0.00
          W          4.00      4.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         15 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         24 Report
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     339.23 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          4 Report
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
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag2A     --S4       .        5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag3A     --S5       .       16.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag4A     --S4       .        5.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1A     --S2       .        8.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1B     --S3       .        6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag1C     --S2       .        7.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag2B     --S4       .        6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag4B     --S1       .       19.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag4B     --S4       .       13.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Ag5A     --O1       .        5.4 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of H6A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6B        Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        33% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  1  )     342.05 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C13 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for        C17 Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C5       - C6       .       1.56 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C10      - C12      .       1.61 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C13      - C14      .       1.58 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C13      - C15      .       1.66 Ang.
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O4             61.2 Degree
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        353 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....              18 Note
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C3A      -H3A1            1_555   1_555 ........     #   92 Check
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PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C2B      -H2B1           1_555   1_555 .......     #  102 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C7       -H7C            1_555   1_555 .......     #  122 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C11      -H11C           1_555   1_555 .......     #  134 Check
PLAT721_ALERT_1_G Bond    Calc     0.97000, Rep     0.96000 Dev...       0.01 Ang.
             C14      -H14C           1_555   1_555 .......     #  141 Check
PLAT722_ALERT_1_G Angle   Calc      145.00, Rep      143.40 Dev...       1.60 Degree
             AG2B    -C6      -H6C        1_555  1_555  1_555     #  340 Check
PLAT722_ALERT_1_G Angle   Calc      145.00, Rep      147.30 Dev...       2.30 Degree
             AG2B    -C6      -H6C        8_556  1_555  1_555     #  341 Check
PLAT722_ALERT_1_G Angle   Calc      106.00, Rep      109.50 Dev...       3.50 Degree
             H6A     -C6      -H6C        1_555  1_555  1_555     #  342 Check
PLAT722_ALERT_1_G Angle   Calc      113.00, Rep      109.50 Dev...       3.50 Degree
             H6B     -C6      -H6C        1_555  1_555  1_555     #  343 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.34 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      31.40 Deg.
             O4   -P1   -C13     1_555   1_555   1_555 ......     #  174 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      42.60 Deg.
             AG5B -S4   -AG5B    8_556   1_555   1_555 ......     #  210 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      31.90 Deg.
             AG2B -S4   -AG2B    8_556   1_555   1_555 ......     #  235 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      33.50 Deg.
             AG2B -S5   -AG2B    8_556   1_555   1_555 ......     #  251 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      41.60 Deg.
             AG5B -S5   -AG5B    4_565   1_555  11_566 ......     #  262 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      35.90 Deg.
             AG2B -C6   -AG2B    1_555   1_555   8_556 ......     #  331 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      37.90 Deg.
             AG2B -C6   -H6B     1_555   1_555   1_555 ......     #  336 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      34.60 Deg.
             AG2B -C12  -AG2B    8_556   1_555   1_555 ......     #  376 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ...      36.80 Deg.
             O4   -C13  -P1      1_555   1_555   1_555 ......     #  380 Check
PLAT794_ALERT_5_G Tentative Bond Valency for W1        (VI)      .       6.06 Info
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       181 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .    Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       77% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....         3 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged    Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         0 Info
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
10 **ALERT level B** = A potentially serious problem, consider carefully
28 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
62 **ALERT level G** = General information/check it is not something unexpected

14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
49 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
26 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.

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

Datablock compound5 - ellipsoid plot