checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: MRMNEa

Bond precision: C-C = 0.0104 A Wavelength=1.54184

Cell: **a=8.6697(3)** **b=15.4417(6)** **c=11.9482(4)**
alpha=90 **beta=99.700(3)** **gamma=90**
Temperature: **285 K**

	Calculated	Reported
Volume	1576.70(10)	1576.70(10)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C30 H46 Ag Cl O P2 S	C30 H46 Ag Cl O P2 S
Sum formula	C30 H46 Ag Cl O P2 S	C30 H46 Ag Cl O P2 S
Mr	660.00	660.03
Dx,g cm-3	1.390	1.390
Z	2	2
Mu (mm-1)	7.636	7.637
F000	688.0	692.3
F000'	692.09	
h,k,lmax	10,19,14	10,19,14
Nref	6384[3315]	5818
Tmin,Tmax	0.101,0.444	0.377,1.994
Tmin'	0.028	

Correction method= GAUSSIAN

Data completeness= 1.76/0.91 **Theta(max)= 73.940**

R(reflections)= 0.0545(5661) **wR2(reflections)= 0.1621(5818)**

S = 1.140 **Npar= Npar = 338**

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low ..... 0.911 Note
PLAT073_ALERT_1_A H-atoms ref, but _hydrogen_treatment reported as constr

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Alert level C
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check

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PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       9.81 Note
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        3.6 Ratio
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............     0.0104 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
             C30 H46 Ag Cl O P2 S
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Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.11 Why ?
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.         46 Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         27 Note
PLAT982_ALERT_1_G The  C-f'=     0.019 Deviates from the  IT-value      0.018
PLAT982_ALERT_1_G The Ag-f'=     0.176 Deviates from the  IT-value      0.131
PLAT982_ALERT_1_G The Cl-f'=     0.368 Deviates from the  IT-value      0.364
PLAT982_ALERT_1_G The  O-f'=     0.052 Deviates from the  IT-value      0.049
PLAT982_ALERT_1_G The  P-f'=     0.304 Deviates from the  IT-value      0.296
PLAT982_ALERT_1_G The  S-f'=     0.335 Deviates from the  IT-value      0.333
PLAT983_ALERT_1_G The Ag-f"=     4.271 Deviates from the  IT-Value      4.282
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   1 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*, 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 05/02/2014; check.def file version of 05/02/2014

Datablock MRMNEa - ellipsoid plot