

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: mrmnea

Bond precision: C-C = 0.0142 Å 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	659.99
Dx, g cm ⁻³	1.390	1.390
Z	2	2
Mu (mm ⁻¹)	7.636	7.636
F000	688.0	688.0
F000'	692.09	
h,k,lmax	10,19,14	10,19,14
Nref	6386[3316]	5818
Tmin,Tmax	0.101,0.444	0.377,1.994
Tmin'	0.028	

Correction method= GAUSSIAN

Data completeness= 1.75/0.91 Theta(max)= 73.945

R(reflections)= 0.0545(5661) wR2(reflections)= 0.1618(5818)

S = 1.138 Npar= Npar = 339

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 C

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	9.78	Note
PLAT220_ALERT_2_C	Large Non-Solvent C Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0142	Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1	Note
C30 H46 Ag Cl O P2 S			



Alert level G

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 ?
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	27 Note

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

0 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
2 ALERT type 3 Indicator that the structure quality may be low
2 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*, 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.

