No syntax errors found.
Please wait while processing ....

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: moc193

Bond precision: C-C = 0.0040 A   Wavelength=0.71073

Cell: a=11.0042(12)   b=12.8657(8)   c=12.5820(12)
             alpha=90   beta=115.436(13) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	1608.7(3)	1608.6(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C13 H11 Ag N4 O7), H2 O	C13 H11 Ag N4 O7, 0.5(H2 O)
Sum formula	C26 H24 Ag2 N8 O15	C13 H12 Ag N4 O7.50
Mr	904.27	452.14
Dx,g cm-3	1.867	1.867
Z	2	4
Mu (mm-1)	1.303	1.303
F000	900.0	900.0
F000'	896.86	
h,k,lmax	14,16,16	14,16,16
Nref	3688	3459
Tmin,Tmax	0.683,0.878	0.715,1.000
Tmin'	0.670	

Correction method= # Reported T Limits: Tmin=0.715
Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.938   Theta(max)= 27.479

R(reflections)= 0.0312(2890)   wR2(reflections)= 0.0789(3459)

S = 1.021   Npar= 240

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full value Low .	0.975	Why?
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	O3B	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N2B	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O1W	0.113	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	73	Report
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.55Ang From O1W .	-0.52	eA-3

And 3 other PLAT976 Alerts

PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.55Ang From O1W .	-0.52	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.68Ang From O1W .	-0.43	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.67Ang From O1W .	-0.40	eA-3

⊠ Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1W Constrained at	0.5	Check

And 2 other PLAT300 Alerts

PLAT300_ALERT_4_G	Atom Site Occupancy of H1WA Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1WB Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	2	Note

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

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   6 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.
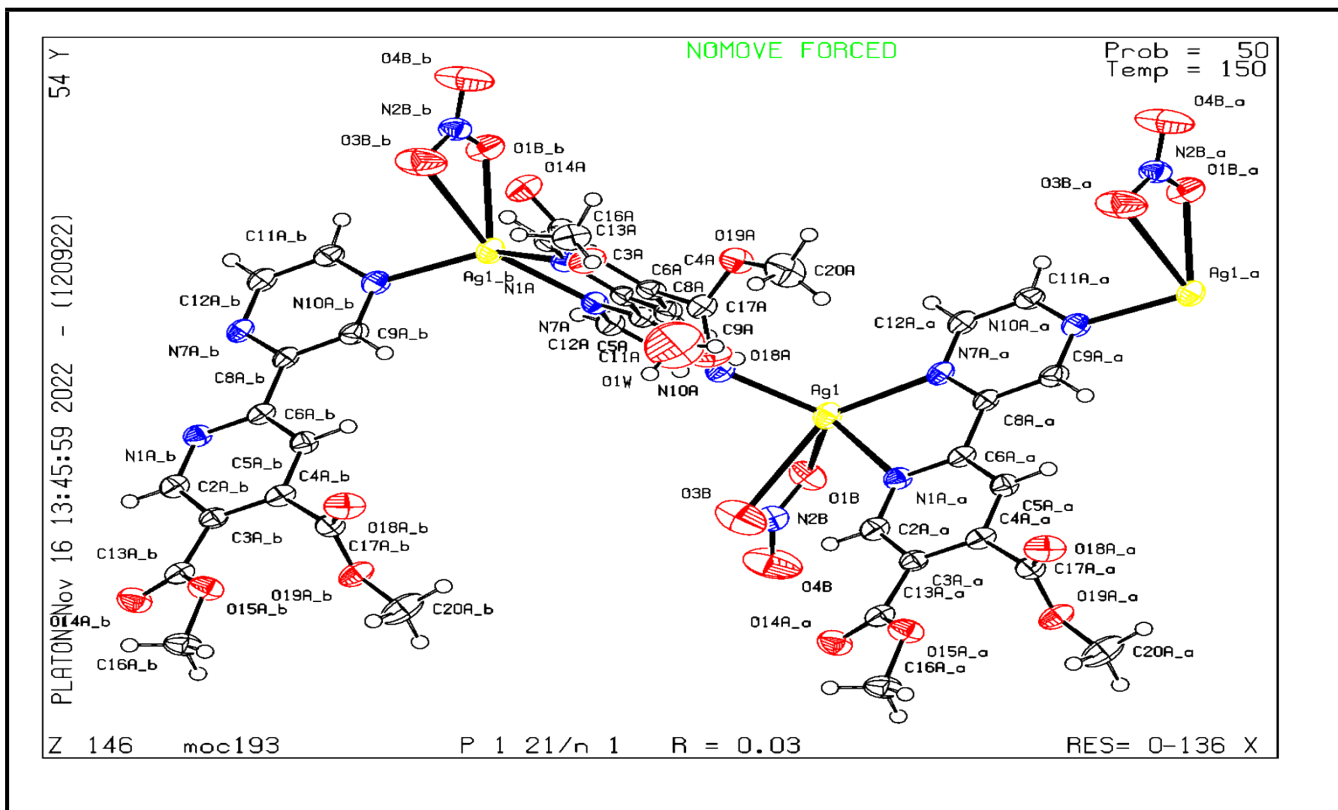
Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 12/09/2022; check.def file version of 09/08/2022

Datablock moc193 - ellipsoid plot