## checkCIF/PLATON (standard)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

# Datablock: 517r

Bond precision: C-C = 0.0172 A Wavelength=0.71073
Cell: a=10.83(2) b=13.90(3) c=13.90(3)
alpha=79.27(2) beta=70.73(2) gamma=70.73(2)
Temperature: 297 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1858(7) | 1859(6) |
| Space group | P -1 | P-1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C21 H24 Ag4 F12 N3 O9 | C21 H24 Ag4 F12 N3 O9 |
| Sum formula | C21 H24 Ag4 F12 N3 O9 | C21 H24 Ag4 F12 N3 O9 |
| Mr | 1121.91 | 1121.91 |
| Dx,g cm-3 | 2.005 | 2.004 |
| Z | 2 | 2 |
| Mu (mm-1) | 2.181 | 2.180 |
| F000 | 1078.0 | 1078.0 |
| F000' | 1071.54 | |
| h,k,lmax | 12,16,16 | 12,16,16 |
| Nref | 6550 | 6486 |
| Tmin,Tmax | 0.514,0.633 | 0.551,0.657 |
| Tmin' | 0.504 | |

Correction method= MULTI-SCAN
Data completeness= 0.990 Theta(max)= 25.000
R(reflections)= 0.0616( 4943) wR2(reflections)= 0.1367( 6486)
S = 1.092 Npar= 573

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

PLAT213_ALERT_2_B Atom F7B has ADP max/min Ratio ..... 4.1 prola
PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 5.3 Ratio
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for O7
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C14
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C16
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C18
PLAT242_ALERT_2_B Check Low Ueq as Compared to Neighbors for C20
PLAT732_ALERT_1_B Angle Calc 70.63(3), Rep 70.63(13) ..... 4.33 su-Ra
AG3 -AG2 -AG1 1.555 1.555 1.555 # 27

### Alert level C

PLAT148_ALERT_3_C su on the a - Axis is (Too) Large ..... 0.020 Ang.
PLAT148_ALERT_3_C su on the b - Axis is (Too) Large ..... 0.030 Ang.
PLAT148_ALERT_3_C su on the c - Axis is (Too) Large ..... 0.030 Ang.
PLAT213_ALERT_2_C Atom F8 has ADP max/min Ratio ..... 3.6 prola
PLAT213_ALERT_2_C Atom C22 has ADP max/min Ratio ..... 3.4 oblat
PLAT213_ALERT_2_C Atom F2 has ADP max/min Ratio ..... 3.4 prola
PLAT213_ALERT_2_C Atom F5 has ADP max/min Ratio ..... 3.4 prola
PLAT213_ALERT_2_C Atom F6 has ADP max/min Ratio ..... 3.6 prola
PLAT213_ALERT_2_C Atom F8B has ADP max/min Ratio ..... 3.6 prola
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 6.0 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag1 -- N1 .. 5.5 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Ag2 -- O9 .. 5.4 su
PLAT234_ALERT_4_C Large Hirshfeld Difference O9 -- C21 .. 0.24 Ang.
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for Ag1
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O1
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for O2
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Ag2
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Ag3
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for N1
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for N2
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C13
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C15
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C17
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C19
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C21
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0172 Ang
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C21 - C22 ... 1.39 Ang.

## Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites .... 1
PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension . 1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..... 0.02000 Deg.
PLAT301_ALERT_3_G Note: Main Residue Disorder ..... 29 Perc.
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms .... !
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints ..... 6

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
29 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
1 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*, 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 18/07/2011; check.def file version of 04/07/2011**

# **Datablock 517r** - ellipsoid plot