checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: sw183

Bond precision: C-C = 0.0032 A   Wavelength=0.71073

Cell:	a=16.8441(2)	b=21.6479(3)	c=19.3995(2)
	alpha=90	beta=92.799(1)	gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	7065.38(15)	7065.38(15)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C116 H100 Ag4 N12 P4, 10(C H2 Cl2), B2 F8, 2(B F4)	C116 H100 Ag4 N12 P4, 10(C H2 Cl2), 4(B F4)
Sum formula	C126 H120 Ag4 B4 Cl20 F16 N12 P4	C126 H120 Ag4 B4 Cl20 F16 N12 P4
Mr	3413.95	3413.95
Dx,g cm-3	1.605	1.605
Z	2	2
Mu (mm-1)	1.043	1.043
F000	3424.0	3424.0
F000'	3424.79	
h,k,lmax	26,33,30	26,33,30
Nref	28231	27393
Tmin,Tmax	0.570,0.785	0.631,0.785
Tmin'	0.559	

Correction method= AbsCorr=MULTI-SCAN

Data completeness= Ratio = 0.970   Theta(max)= 33.730

R(reflections)= 0.0398(18240)   wR2(reflections)= 0.0952(27393)

S = 0.923   Npar= 978

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   F3A   -- F3B   ..   8.36 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ag1   -- P1   ..   23.76 su
PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Ag2   -- P1   ..   19.70 su
PLAT241_ALERT_2_B Check High   Ueq as Compared to Neighbors for   F3B

```
PLAT242_ALERT_2_B Check Low        Ueq as Compared to Neighbors for        B1A
```

___

🟡 **Alert level C**

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.97
PLAT220_ALERT_2_C Large Non-Solvent    C     Ueq(max)/Ueq(min) ...      3.02 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F1A    -- F1B    ..        6.63 su
PLAT241_ALERT_2_C Check High       Ueq as Compared to Neighbors for       F1B
PLAT241_ALERT_2_C Check High       Ueq as Compared to Neighbors for       F2B
PLAT241_ALERT_2_C Check High       Ueq as Compared to Neighbors for       F4A
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.79
PLAT301_ALERT_3_C Main Residue  Disorder ........................      3.00 Perc.
PLAT431_ALERT_2_C Short Inter HL..A Contact Cl4    .. N200    ..        3.19 Ang.
PLAT431_ALERT_2_C Short Inter HL..A Contact F8     .. Cl6B    ..        3.04 Ang.
PLAT042_ALERT_1_C Calc. and Rep. MoietyFormula Strings Differ ....        ?
PLAT060_ALERT_4_C Ratio Tmax/Tmin (Exp-to-Rep) (too) Large .......      1.11
PLAT243_ALERT_4_C High  'Solvent' Ueq as Compared to Neighbors for      C3SA
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors for      C1SB
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors for      C1SA
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors for      C5SB
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors for      C3SB
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors for      C4SB
PLAT720_ALERT_4_C Number of Unusual/Non-Standard Labels ..........        26
```

___

⚪ **Alert level G**

```
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......        4
PLAT302_ALERT_4_G Anion/Solvent Disorder ........................      38.00 Perc.
PLAT793_ALERT_4_G Check the Absolute Configuration of P2     .....        S
```

___

```
  0 ALERT level A = In general: serious problem
  5 ALERT level B = Potentially serious problem
 19 ALERT level C = Check and explain
  3 ALERT level G = General alerts; check

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 13 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
 10 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
```

___

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.

Datablock sw183 - ellipsoid plot