checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: dl205b

Bond precision: C-C = 0.0041 A   Wavelength=0.71073

Cell: a=10.4930(4)   b=18.9540(9)   c=14.2810(6)
                 alpha=90   beta=100.992(4)   gamma=90
Temperature: 180 K

	Calculated	Reported
Volume	2788.2(2)	2788.2(2)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C25 H30 N2 P, C H2 Cl2, I	C25 H30 N2 P, C H2 Cl2, I
Sum formula	C26 H32 Cl2 I N2 P	C26 H32 Cl2 I N2 P
Mr	601.31	601.31
Dx,g cm-3	1.433	1.432
Z	4	4
Mu (mm-1)	1.414	1.414
F000	1216.0	1216.0
F000'	1216.00	
h,k,lmax	13,23,17	13,23,17
Nref	5694	5683
Tmin,Tmax	0.749,0.893	0.661,0.885
Tmin'	0.654	

Correction method= MULTI-SCAN

Data completeness= 0.998   Theta(max)= 26.370

R(reflections)= 0.0288(3596)   wR2(reflections)= 0.0581(5683)

S = 0.902   Npar= 293

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**

PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #   2
            C H2 Cl2
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #   3
            I

Alert level G

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PLAT128_ALERT_4_G Non-standard setting of Space-group P21/c   ....       P21/n
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =         3
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   0 ALERT level A = In general: serious problem
   0 ALERT level B = Potentially serious problem
   2 ALERT level C = Check and explain
   2 ALERT level G = General alerts; check

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   4 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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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 13/08/2009; check.def file version of 12/08/2009