checkCIF/PLATON report

No syntax errors found.   **CIF dictionary**   **Interpreting this report**

Datablock: phw1114

Bond precision: C-C = 0.0041 A   Wavelength=0.71070

Cell: a=14.3660(6)   b=14.5323(7)   c=15.0613(6)
              alpha=88.273(4)   beta=63.679(4)   gamma=71.691(4)

Temperature: 110 K

	Calculated	Reported
Volume	2653.6(2)	2653.6(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C21 H30 N6), 3(C H Cl3)	2(C21 H30 N6), 3(C H Cl3)
Sum formula	C45 H63 Cl9 N12	C45 H63 Cl9 N12
Mr	1091.12	1091.12
Dx,g cm-3	1.366	0.000
Z	2	2
Mu (mm-1)	0.520	0.520
F000	1140.0	1188.0
F000'	1142.92	
h,k,lmax	19,19,20	19,19,20
Nref	14234	11934
Tmin,Tmax	0.963,0.981	0.906,0.984
Tmin'	0.890	

Correction method= ANALYTICAL

Data completeness= 0.838   Theta(max)= 29.090

R(reflections)= 0.0565(8395)   wR2(reflections)= 0.1191(11934)

S = 1.018   Npar= 643

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 A
TYPE027_ALERT_1_A _exptl_crystal_density_diffrn is not of type numb.
DENSD01_ALERT_1_A The ratio of the submitted crystal density and that
          calculated from the formula is outside the range 0.90 <> 1.10
          Crystal density given   =   1.000
          Calculated crystal density =   1.365

Alert level C

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PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...        ? Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of      C44
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.0041 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact  H27A   ..  H27A    ..    2.03 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor        N1    -  H1A    ...        ? Check
PLAT420_ALERT_2_C D-H Without Acceptor        N2    -  H2     ...        ? Check
PLAT420_ALERT_2_C D-H Without Acceptor        N3    -  H3A    ...        ? Check
PLAT420_ALERT_2_C D-H Without Acceptor        N7    -  H7     ...        ? Check
PLAT420_ALERT_2_C D-H Without Acceptor        N8    -  H8     ...        ? Check
PLAT420_ALERT_2_C D-H Without Acceptor        N9    -  H9A    ...        ? Check
PLAT420_ALERT_2_C D-H Without Acceptor        N11   -  H11A   ...        ? Check
PLAT420_ALERT_2_C D-H Without Acceptor        N12   -  H12    ...        ? Check
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Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF       ? Do !
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal .........  0.00400 Deg.
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   2 ALERT level G = General information/check it is not something unexpected

   4 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
   1 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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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 01/06/2013; check.def file version of 24/05/2013

NOMOVE FORCED

Prob = 50
Temp = 110

43 Y

PLATON-Jun 14 15:58:25 2013 - (100912)

Z 176   phw1114   P -1   R = 0.06   RES= 0   -75 X