checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: phw1115

Bond precision: C-C = 0.0028 A   Wavelength=0.71070

Cell: a=13.8281(3)   b=13.8281(3)   c=8.2311(2)
               alpha=90   beta=90   gamma=120
Temperature: 110 K

	Calculated	Reported
Volume	1363.06(8)	1363.07(6)
Space group	P 3 1 c	P 3 1 c
Hall group	P 3 -2c	P 3 -2c
Moiety formula	C27 H30 Cl3 N3 O3	C27 H30 Cl3 N3 O3
Sum formula	C27 H30 Cl3 N3 O3	C27 H30 Cl3 N3 O3
Mr	550.89	550.89
Dx,g cm-3	1.342	1.342
Z	2	2
Mu (mm-1)	0.370	0.370
F000	576.0	576.0
F000'	577.09	
h,k,lmax	20,20,12	20,20,12
Nref	3239[1628]	2940
Tmin,Tmax	0.938,0.958	0.966,0.984
Tmin'	0.893	

Correction method= ANALYTICAL

Data completeness= 1.81/0.91   Theta(max)= 32.270

R(reflections)= 0.0404(2681)   wR2(reflections)= 0.1057(2940)

S = 1.111   Npar= 117

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**
PLAT245_ALERT_2_C U(iso) H1A   Smaller than U(eq) N1   by ...   0.011 AngSq
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .   63 Ang3
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #   1
              C27 H30 Cl3 N3 O3

Alert level G

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PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF          ? Do !
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...        2 Units
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   2 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
   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

PLATON-Jun 14 12:14:54 2013 - (100912)

Z -25   phw1115   P 3 1 c   R = 0.04   RES= 0   0 X