checkCIF/PLATON report

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

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

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Bond precision:  C-C = 0.0127 A          Wavelength=0.71073

Cell:          a=10.0618(3)      b=10.1653(3)     c=27.0304(11)
               alpha=87.163(1)   beta=85.001(1)   gamma=66.509(1)
Temperature:   120 K
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	Calculated	Reported
Volume	2525.60(15)	2525.60(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H40 Cd N4 O2, C15 H18 N2, 2(Cl O4), C2 H6 O	C30 H40 Cd N6 O2, C15 H18 N2, 2(Cl O4), C2 H6 O
Sum formula	C47 H64 Cd Cl2 N6 O11	C47 H64 Cd Cl2 N6 O11
Mr	1072.35	1072.34
Dx,g cm-3	1.410	1.410
Z	2	2
Mu (mm-1)	0.601	0.601
F000	1116.0	1116.0
F000’	1115.44	
h,k,lmax	12,12,33	12,12,33
Nref	9941	9645
Tmin,Tmax	0.951,0.970	0.942,0.971
Tmin’	0.942	

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Correction method= # Reported T Limits: Tmin=0.942 Tmax=0.971
AbsCorr = MULTI-SCAN

Data completeness= 0.970          Theta(max)= 26.000

R(reflections)= 0.0908( 6116)     wR2(reflections)= 0.2206( 9645)

S = 1.097                 Npar= 608
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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

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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.135
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 .....      0.135 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....    2.19 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference C312   --  C313    ..    0.18 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............  0.0127 Ang.
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and _chemical_formula_moiety. This is
           usually due to the moiety formula being in the wrong format.
           Atom count from _chemical_formula_sum:   C47 H64 Cd1 Cl2 N6 O11
           Atom count from _chemical_formula_moiety:C47 H64 Cd1 Cl2 N8 O11
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          4 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          5 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      20.69 Why ?
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..........    0.00100 Degree
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of         Cl1 Check
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of         Cl2 Check
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          3 Do !
           N11 -CD1 -N11 -C105 -165.00  5.00   2.655   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #          8 Do !
           N11 -CD1 -N11 -C101   37.00  5.00   2.655   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         15 Do !
           N12 -CD2 -N12 -C113  -95.00 26.00   2.566   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         20 Do !
           N12 -CD2 -N12 -C114   78.00 26.00   2.566   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         53 Do !
           N21 -CD1 -N21 -C201 -107.00 15.00   2.655   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #         58 Do !
           N21 -CD1 -N21 -C205   61.00 15.00   2.655   1.555   1.555   1.555
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         24 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
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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
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  19 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  10 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 29/01/2015; check.def file version of 29/01/2015

Datablock I - ellipsoid plot