checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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

Bond precision: C-C = 0.0042 A Wavelength=0.71073

Cell: a=11.0586(3) b=23.5007(6) c=17.3454(5)
alpha=90 beta=105.627(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4341.2(2)	4341.2(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C48 H33 Cd N6 O4	Cd (C12 H10 N4)1.5 (C15 H9 O2)2, C H4 O
Sum formula	C48 H33 Cd N6 O4	C49 H37 Cd N6 O5
Mr	870.21	902.24
Dx,g cm-3	1.332	1.380
Z	4	4
Mu (mm-1)	0.553	0.557
F000	1772.0	1844.0
F000’	1769.42	
h,k,lmax	14,30,22	14,30,22
Nref	10101	10043
Tmin,Tmax	0.818,0.895	0.865,0.912
Tmin’	0.800	

Correction method= GAUSSIAN

Data completeness= 0.994 Theta(max)= 27.627

R(reflections)= 0.0360(8862) wR2(reflections)= 0.0961(10043)

S = 1.077 Npar= 532

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

PLAT015_ALERT_5_A No _shelx_hkl_file record in SHELXL20xy CIF ... Please Do !

Author Response: File is too large.

Alert level B

Crystal system given = monoclinic
PLAT910_ALERT_3_B Missing # of FCF Reflections Below Th(Min) ..... 13 Report

---

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as Gaussian
CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as
calculated from the _atom_site* data lies outside
the range 0.99 <> 1.01
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_weight 902.24
TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
C	12.01	48.00	576.53
H	1.01	33.00	33.26
N	14.01	6.00	84.04
O	16.00	4.00	64.00
Cd	112.41	1.00	112.41

Calculated formula weight 870.24
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... O2 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... N4 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.786 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 12 Report

---

Alert level G

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: C49 H37 Cd1 N6 O5
Atom count from _chemical_formula_moiety:C1 H4 O1
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C49 H37 Cd1 N6 O5
Atom count from the _atom_site data: C48 H33 Cd1 N6 O4
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C49 H37 Cd N6 O5
TEST: Compare cell contents of formula and atom_site data

```
           atom    Z*formula  cif sites diff
           C        196.00    192.00    4.00
           H        148.00    132.00   16.00
           Cd         4.00      4.00    0.00
           N         24.00     24.00    0.00
           O         20.00     16.00    4.00
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension .......          2 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT044_ALERT_1_G Calculated and Reported Density Dx  Differ by ..     0.0485 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd1    --  O1      ..       11.8 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd1    --  O2      ..        9.7 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Cd1    --  O4      ..        7.1 su
PLAT605_ALERT_4_G Structure Contains Solvent Accessible VOIDS of .        295 A**3
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          16 Info
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         34 Note
```

```
   1 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 24/07/2014; check.def file version of 24/07/2014

Datablock I - ellipsoid plot