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: 3

Bond precision: C-C = 0.0050 A Wavelength=0.71073

Cell: a=7.4629(2) b=24.0425(6) c=18.6052(4)
alpha=90 beta=92.373(2) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	3335.41(14)	3335.41(14)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C18 H24 Cd N6 O6, C6 H6 N2 O, 2(Cl O4)	?
Sum formula	C24 H30 Cd Cl2 N8 O15	C24 H30 Cd Cl2 N8 O15
Mr	853.87	853.86
Dx,g cm-3	1.700	1.700
Z	4	4
Mu (mm-1)	0.896	0.896
F000	1728.0	1728.0
F000'	1726.83	
h,k,lmax	8,28,22	8,28,22
Nref	5862	5834
Tmin,Tmax		0.842,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.842 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 24.998

R(reflections)= 0.0344(4760) wR2(reflections)= 0.1002(5834)

S = 1.048 Npar= 493

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

```
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.95 Report
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Cd1      --O6       .        6.3 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Cd1 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl2      0.132 Check
PLAT314_ALERT_2_C Small Angle for H2O: Metal-O6       -H26O      .      63.34 Degree
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N4       --H14N     .     Please Check
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         21 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         14 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          3 Report
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
PLAT303_ALERT_2_G Full Occupancy Atom H26O      with # Connections       2.00 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
              C6 H6 N2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          3 Note
              Cl O4
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1       (II)      .       2.31 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        17 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.2 Low
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       50.0 Degree
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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
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
   6 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT053_3
;
PROBLEM: Minimum Crystal Dimension Missing (or Error) ...     Please Check
```

```
RESPONSE: ...
;
_vrf_PLAT054_3
;
PROBLEM: Medium  Crystal Dimension Missing (or Error) ...     Please Check
RESPONSE: ...
;
_vrf_PLAT055_3
;
PROBLEM: Maximum Crystal Dimension Missing (or Error) ...     Please Check
RESPONSE: ...
;
_vrf_PLAT094_3
;
PROBLEM: Ratio of Maximum / Minimum Residual Density ....       2.95 Report
RESPONSE: ...
;
_vrf_PLAT232_3
;
PROBLEM: Hirshfeld Test Diff (M-X)  Cd1      --O6       .        6.3 s.u.
RESPONSE: ...
;
_vrf_PLAT242_3
;
PROBLEM: Low    'MainMol' Ueq as Compared to Neighbors of        Cd1 Check
RESPONSE: ...
;
_vrf_PLAT260_3
;
PROBLEM: Large Average Ueq of Residue Including       Cl2      0.132 Check
RESPONSE: ...
;
_vrf_PLAT314_3
;
PROBLEM: Small Angle for H2O: Metal-O6       -H26O      .      63.34 Degree
RESPONSE: ...
;
_vrf_PLAT420_3
;
PROBLEM: D-H Bond Without Acceptor  N4       --H14N     .     Please Check
RESPONSE: ...
;
# end Validation Reply Form
```

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* or *IUCrData*, 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 28/11/2022; check.def file version of 28/11/2022

Datablock 3 - ellipsoid plot