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: 1_sq_pl

```
Bond precision:   C-C = 0.0035 A          Wavelength=0.71073

Cell:             a=15.647(5)     b=8.296(3)          c=14.600(5)
                  alpha=90        beta=94.992(4)      gamma=90
Temperature:      298 K
```

	Calculated	Reported
Volume	1888.0(11)	1888.0(11)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C15 H16 Cd N O6, Cl O4, H2 O	C15 H16 Cd N O6, Cl O4, H2 O
Sum formula	C15 H18 Cd Cl N O11	C15 H18 Cd Cl N O11
Mr	536.16	536.15
Dx,g cm-3	1.886	1.886
Z	4	4
Mu (mm-1)	1.360	1.360
F000	1072.0	1072.0
F000'	1069.97	
h,k,lmax	20,11,19	20,10,19
Nref	4661	4394
Tmin,Tmax	0.640,0.838	0.735,1.000
Tmin'	0.624	

```
Correction method= # Reported T Limits: Tmin=0.735 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.943           Theta(max)= 28.216

R(reflections)= 0.0285( 3815)                    wR2(reflections)=
                                                 0.0743( 4394)
S = 1.057                  Npar= 270
```

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

PLAT230_ALERT_2_C Hirshfeld Test Diff for O4 --C9_c . 5.2 s.u.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 6 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cd1 --O2 . 8.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cd1 --O3 . 5.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cd1 --O6 . 7.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cd1 --O4_c . 19.2 s.u.
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of Cl1 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1 (II) . 2.06 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 2.8 Low

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **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

0 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
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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 18/05/2022; check.def file version of 17/05/2022

Datablock 1_sq_pl - ellipsoid plot