

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 411-13Cd

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: 411-13Cd

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Bond precision:	C-C = 0.0158 A	Wavelength=0.71073
Cell:	a=7.1639(3)      b=17.8025(8)      c=26.3248(10)	alpha=90      beta=93.142(4)      gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	3352.3(2)	3352.3(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C36 H24 Cd2 N4 O10	?
Sum formula	C36 H24 Cd2 N4 O10	C36 H24 Cd2 N4 O10
Mr	897.41	897.39
Dx,g cm-3	1.778	1.778
Z	4	4
Mu (mm-1)	1.335	1.335
F000	1776.0	1776.0
F000'	1770.33	
h,k,lmax	8,21,31	8,21,31
Nref	5951	5932
Tmin,Tmax	0.733,0.756	0.740,0.767
Tmin'	0.719	

Correction method= # Reported T Limits: Tmin=0.740 Tmax=0.767  
AbsCorr = MULTI-SCAN

Data completeness= 0.997      Theta(max)= 25.050

R(reflections)= 0.0662( 4028)      wR2(reflections)= 0.1595( 5932)

S = 1.020      Npar= 470

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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.

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**Alert level B**

PLAT910\_ALERT\_3\_B Missing # of FCF Reflection(s) Below Theta(Min). 17 Note

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**Alert level C**

PLAT220\_ALERT\_2\_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 5.0 Ratio  
PLAT220\_ALERT\_2\_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 4.5 Ratio  
PLAT222\_ALERT\_3\_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 4.2 Ratio  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Cd2 --O10 . 0.16 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C15 --C16 . 0.18 Ang.  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 03 Check  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 05 Check  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 06 Check  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 07 Check  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C12 Check  
PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C34 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of Cd2 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C11 Check  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C16 Check  
PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including Cd1 0.077 Check  
PLAT314\_ALERT\_2\_C Small Angle for H2O: Metal-O10 -H1W . 83.02 Degree  
PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.01582 Ang.  
PLAT369\_ALERT\_2\_C Long C(sp2)-C(sp2) Bond C11 - C12 . 1.53 Ang.  
PLAT430\_ALERT\_2\_C Short Inter D...A Contact O1 ..04 . 2.90 Ang.  
-1+x,y,z = 1\_455 Check  
PLAT480\_ALERT\_4\_C Long H...A H-Bond Reported H17 ..03 . 2.64 Ang.  
PLAT480\_ALERT\_4\_C Long H...A H-Bond Reported H1W ..08 . 2.64 Ang.  
PLAT480\_ALERT\_4\_C Long H...A H-Bond Reported H17 ..03 . 2.64 Ang.  
PLAT480\_ALERT\_4\_C Long H...A H-Bond Reported H1W ..08 . 2.64 Ang.  
PLAT480\_ALERT\_4\_C Long H...A H-Bond Reported H17 ..03 . 2.64 Ang.  
PLAT480\_ALERT\_4\_C Long H...A H-Bond Reported H1W ..08 . 2.64 Ang.  
PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 5.511 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.596 2 Report  
PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 2.34A From O7 1.75 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 1.07A From O7 0.75 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.98A From O8 0.42 eA-3  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.83A From O7 -0.77 eA-3  
PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 0.92A From O6 -0.42 eA-3  
PLAT978\_ALERT\_2\_C Number C-C Bonds with Positive Residual Density. 0 Info

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**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 2 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 3 Report  
PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 3 Info  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 2 Report  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 19.00 Why ?  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
PLAT177\_ALERT\_4\_G The CIF-Embedded .res File Contains DELU Records 1 Report  
PLAT178\_ALERT\_4\_G The CIF-Embedded .res File Contains SIMU Records 1 Report  
PLAT199\_ALERT\_1\_G Reported \_cell\_measurement\_temperature .... (K) 293 Check  
PLAT200\_ALERT\_1\_G Reported \_diffrn\_ambient\_temperature .... (K) 293 Check  
PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) Cd2 --O7 . 19.9 s.u.  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Cd1 (II) . 2.02 Info  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Cd2 (II) . 2.19 Info  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 16 Note  
PLAT909\_ALERT\_3\_G Percentage of I>2sig(I) Data at Theta(Max) Still 38% Note  
PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 1 Note

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0 ALERT level A = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully  
33 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
16 **ALERT level G** = General information/check it is not something unexpected

2 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data  
25 **ALERT type 2** Indicator that the structure model may be wrong or deficient  
8 **ALERT type 3** Indicator that the structure quality may be low  
11 **ALERT type 4** Improvement, methodology, query or suggestion  
4 **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* 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.

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**PLATON version of 19/10/2018; check.def file version of 15/10/2018**

