

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: bcd35a_0m

Bond precision: C-C = 0.0027 Å Wavelength=0.71073

Cell: a=9.5015(3) b=9.5015(3) c=65.063(3)
 alpha=90 beta=90 gamma=120
Temperature: 296 K

	Calculated	Reported
Volume	5086.9(5)	5086.9(3)
Space group	R -3 c	R-3c
Hall group	-R 3 2" c	?
Moiety formula	C36 H36 Cd N6, 2(C1 O4)	C36 H36 Cd N6, 2(C1 O4)
Sum formula	C36 H36 Cd Cl2 N6 O8	C36 H36 Cd Cl2 N6 O8
Mr	864.02	864.01
Dx,g cm-3	1.692	1.692
Z	6	6
Mu (mm-1)	0.867	0.867
F000	2640.0	2640.0
F000'	2637.99	
h,k,lmax	12,12,87	12,12,86
Nref	1443	1439
Tmin,Tmax	0.856,0.909	0.853,0.911
Tmin'	0.848	

Correction method= # Reported T Limits: Tmin=0.853 Tmax=0.911
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 28.490

R(reflections)= 0.0261(1241) wR2(reflections)= 0.1149(1439)

S = 0.942 Npar= 81

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

PLAT430_ALERT_2_A Short Inter D...A Contact 01 .. 01 .. 2.31 Ang.
PLAT430_ALERT_2_A Short Inter D...A Contact 01 .. 01 .. 2.31 Ang.

Alert level B

SYMMS02_ALERT_1_B The unit-cell lengths a and c should be equal for a rhombohedral cell

Cell 9.5015 9.5015 65.0630
Angles 90.0000 90.0000 120.0000

SYMMS02_ALERT_1_B Cell angles alpha and gamma should be equal for a rhombohedral cell

Cell 9.5015 9.5015 65.0630
Angles 90.0000 90.0000 120.0000

SYMMS02_ALERT_1_B All angles should not be 90 for a rhombohedral cell

Cell 9.5015 9.5015 65.0630
Angles 90.0000 90.0000 120.0000

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as . mixed Check
PLAT104_ALERT_1_G The Reported Crystal System is Inconsistent with R-3c Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 2 Units
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of Cl1 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl1 .. 01 .. 1.42 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl1 .. 01 .. 1.42 Ang.
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # 5 Do !
N1 -CD1 -N1 -C1 -28.40 1.10 19.775 1.555 1.555 1.555
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON 185 Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 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

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 21/06/2015; check.def file version of 21/06/2015

