

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

Bond precision: C-C = 0.0071 Å

Wavelength=0.71073

Cell: a=15.0305(14) b=7.2772(6) c=11.8887(10)
 alpha=90 beta=101.986(3) gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	1272.04(19)	1272.03(19)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	C22 H32 Cd N6 O6	?
Sum formula	C22 H32 Cd N6 O6	C2.93 H4.27 Cd0.13 N0.80 O0.80
Mr	588.95	78.52
Dx, g cm ⁻³	1.538	1.538
Z	2	15
Mu (mm ⁻¹)	0.907	0.907
F000	604.0	604.0
F000'	602.62	
h, k, lmax	19, 9, 15	19, 9, 15
Nref	2832	2929
Tmin, Tmax	0.849, 0.913	0.789, 0.820
Tmin'	0.834	

Correction method= # Reported T Limits: Tmin=0.789 Tmax=0.820
AbsCorr = MULTI-SCAN

Data completeness= 1.034

Theta(max)= 27.200

R(reflections)= 0.0377(2251)

wR2(reflections)= 0.1084(2929)

S = 1.091

Npar= 157

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

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies
outside the range 0.99 <> 1.01
Calculated value of mu = 0.886
Value of mu given = 0.907
PLAT021_ALERT_4_C Ratio Unique / Expected Reflections too High ... 1.034
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.10 Report
PLAT165_ALERT_3_C Nr. of Status R Flagged Non-Hydrogen Atoms 1 Note
PLAT230_ALERT_2_C Hirshfeld Test Diff for O2 -- C11 .. 6.8 s.u.
PLAT410_ALERT_2_C Short Intra H...H Contact H4 .. H6B .. 1.97 Ang.

● Alert level G

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 15
From the CIF: _chemical_formula_sum C2.93 H4.27 Cd0.13 N0.80 O0.80
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	43.95	44.00	-0.05
H	64.05	64.00	0.05
Cd	1.95	2.00	-0.05
N	12.00	12.00	0.00
O	12.00	12.00	0.00

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 2 Report
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.13 Check
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints 12 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

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

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

