

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: I

Bond precision: C-C = 0.0062 Å Wavelength=0.71073

Cell: a=17.7584(5) b=9.8785(3) c=12.3847(4)
 alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	2172.60(11)	2172.60(11)
Space group	P n a 21	P n a 2(1)
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C16 H15 Cd Cl N6 O5, Cl 04	[CD(2,2
Sum formula	C16 H15 Cd Cl2 N6 O9	C16 H16 Cd Cl2 N6 O9
Mr	618.65	619.65
Dx, g cm-3	1.891	1.894
Z	4	4
Mu (mm-1)	1.314	1.315
F000	1228.0	1232.0
F000'	1226.51	
h, k, lmax	21, 11, 14	21, 11, 14
Nref	3842[2018]	3304
Tmin, Tmax	0.802, 0.854	0.802, 0.854
Tmin'	0.800	

Correction method= # Reported T Limits: Tmin=0.802 Tmax=0.854
AbsCorr = MULTI-SCAN

Data completeness= 1.64/0.86 Theta(max)= 25.030

R(reflections)= 0.0267(3118) wR2(reflections)= 0.0639(3304)

S = 1.007 Npar= 307

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

HYDTR01_ALERT_1_C The hydrogen treatment should only be one of the following

keywords
* refall
* refxyz
* refU
* noref
* undef
* constr
* none
* mixed
* hetero
* heteroxyz
* heteroU
* heteronoref
* hetero-mixed
* heteroxyz-mixed
* heteroU-mixed
* heteronoref-mixed

Hydrogen treatment given as theo

STRVA01_ALERT_4_C Flack test results are meaningless.

From the CIF: _refine_ls_abs_structure_Flack 0.000

From the CIF: _refine_ls_abs_structure_Flack_su 10.000

PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ	Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..	1.00 Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	6.57 Note
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
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N5 Check

● Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the

_chemical_formula_sum and _chemical_formula_moiety. This is usually due to the moiety formula being in the wrong format.

Atom count from _chemical_formula_sum: C16 H16 Cd1 Cl2 N6 O9

Atom count from _chemical_formula_moiety:

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the _chemical_formula_sum and the formula from the _atom_site* data.

Atom count from _chemical_formula_sum: C16 H16 Cd1 Cl2 N6 O9

Atom count from the _atom_site data: C16 H15 Cd1 Cl2 N6 O9

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_sum C16 H16 Cd Cl2 N6 O9

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	64.00	64.00	0.00
H	64.00	60.00	4.00
Cd	4.00	4.00	0.00
Cl	8.00	8.00	0.00
N	24.00	24.00	0.00
O	36.00	36.00	0.00

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	3 Report
PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High .	10.000 Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check

PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	(K)	293	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C12	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		C11	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		1	Note
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 and s.u.		10.00	Check
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL		2016	Note

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
 17 **ALERT level G** = General information/check it is not something unexpected

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

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
 _publ_contact_author_name and _publ_contact_author_address.
 PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
 _publ_contact_author_phone are all missing.
 At least one of these should be present.
 PUBL006_ALERT_1_A _publ_requested_journal is missing
 e.g. 'Acta Crystallographica Section C'
 PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
 PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
 PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
 PUBL012_ALERT_1_A _publ_section_abstract is missing.
 Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or
 empty.

7 **ALERT level A** = Data missing that is essential or data in wrong format
 1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
```

PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 13/08/2017; check.def file version of 27/07/2017

Datablock 1 - ellipsoid plot

