

# 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: Compound2

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Bond precision:    C-C = 0.0050 A

Wavelength=0.71069

Cell:                a=8.7080(4)                b=9.0640(3)                c=19.4510(7)  
                      alpha=101.089(1)        beta=90.961(2)        gamma=98.063(1)  
Temperature:        100 K

	Calculated	Reported
Volume	1490.18(10)	1490.18(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C32 H20 Cd2 N8 O8	?
Sum formula	C32 H20 Cd2 N8 O8	C32 H20 Cd2 N8 O8
Mr	869.38	869.36
Dx,g cm-3	1.938	1.937
Z	2	2
Mu (mm-1)	1.497	1.497
F000	856.0	856.0
F000'	853.11	
h,k,lmax	11,12,26	11,12,26
Nref	7720	7671
Tmin,Tmax	0.811,0.823	0.702,0.746
Tmin'	0.811	

Correction method= # Reported T Limits: Tmin=0.702 Tmax=0.746  
AbsCorr = EMPIRICAL

Data completeness= 0.994

Theta(max)= 28.736

R(reflections)= 0.0352( 5938)

wR2(reflections)= 0.0823( 7671)

S = 1.109

Npar= 451

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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.



## Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	4	Report
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3	Note
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	4	Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.11	Ratio
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd1 (II) .	1.97	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd2 (II) .	2.01	Info
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	8	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	6	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 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  
4 ALERT type 4 Improvement, methodology, query or suggestion  
5 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

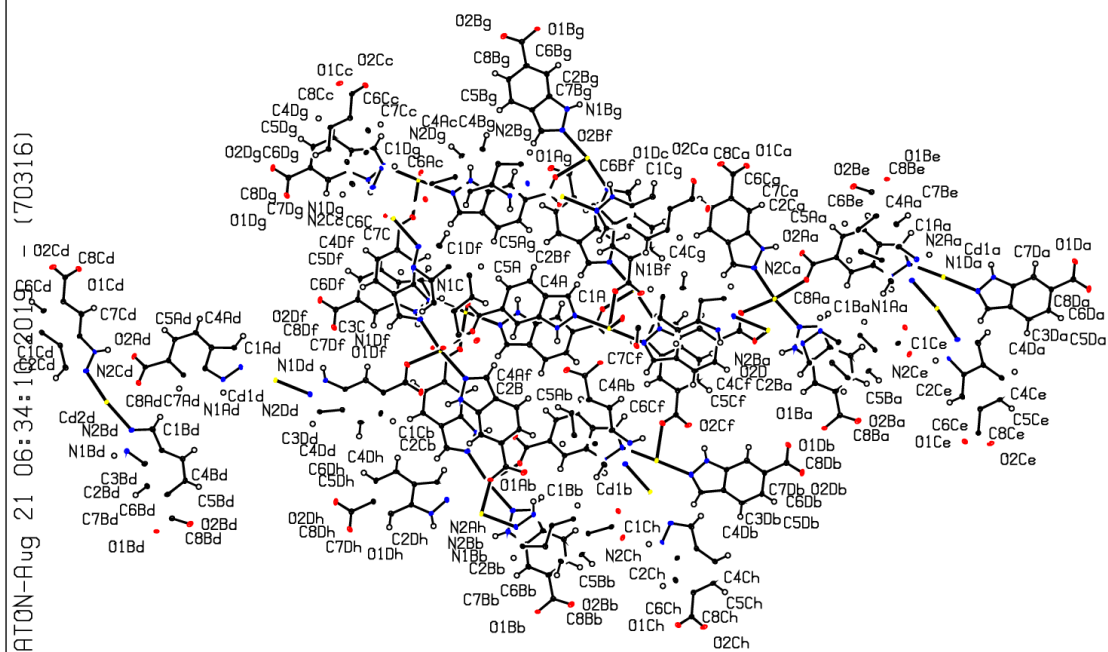
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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Prob = 50
Temp = 100

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Z 114

Compound2 P -1

$$R = 0.04$$

RES= 0 -132 X