

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

Bond precision: C-C = 0.0039 A Wavelength=0.71073

Cell: a=11.810(1) b=13.7340(12) c=22.809(2)

 alpha=90 beta=95.290(1) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	3683.8(6)	3683.8(6)
Space group	P 2/c	P2/c
Hall group	-P 2yc	?
Moiety formula	C72 H62 Cd N10, 2(C6 H2 N3 O7)	?
Sum formula	C84 H66 Cd N16 O14	C84 H66 Cd N16 O14
Mr	1635.94	1635.93
Dx,g cm-3	1.475	1.475
Z	2	2
Mu (mm-1)	0.378	0.378
F000	1684.0	1684.0
F000'	1683.10	
h,k,lmax	14,16,27	14,16,27
Nref	6868	6866
Tmin,Tmax	0.860,0.893	0.860,0.893
Tmin'	0.860	

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.500

R(reflections)= 0.0365(6091) wR2(reflections)= 0.1000(6866)

S = 1.045 Npar= 519

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 B

PLAT242_ALERT_2_B Check Low

Ueq as Compared to Neighbors for

N8



Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.06
PLAT213_ALERT_2_C	Atom O7 has ADP max/min Ratio	3.4 prola
PLAT220_ALERT_2_C	Large Non-Solvent O Ueq(max)/Ueq(min) ...	3.3 Ratio
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for	N6
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.1



Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	?
PLAT194_ALERT_1_G	Missing _cell_measurement_reflms_used datum	?
PLAT195_ALERT_1_G	Missing _cell_measurement_theta_max datum	?
PLAT196_ALERT_1_G	Missing _cell_measurement_theta_min datum	?
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature	293 K

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 6 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
 0 ALERT type 4 Improvement, methodology, query or suggestion
 1 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.

Datablock 1 - ellipsoid plot

