

Supplementary material for the article:

Ristovic, M. S.; Zianna, A.; Psomas, G.; Hatzidimitriou, A. G.; Coutouli-Argyropoulou, E.; Lalia-Kantouri, M. Interaction of Dinuclear Cadmium(II) 5-Cl-Salicylaldehyde Complexes with Calf-Thymus DNA. *Materials Science and Engineering C* **2016**, *61*, 579–590.

<https://doi.org/10.1016/j.msec.2015.12.054>

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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 = 0.0103 Å Wavelength=0.71073

Cell: a=7.5156(7) b=27.071(3) c=8.1433(7)
 alpha=90 beta=91.438(4) gamma=90

Temperature: 295 K

	Calculated	Reported
Volume	1656.3(3)	1656.27(14)
Space group	P 21/a	P 21/a
Hall group	-P 2yab	?
Moiety formula	C30 H24 Cd2 Cl4 O10	C30 H24 Cd2 Cl4 O10
Sum formula	C30 H24 Cd2 Cl4 O10	C30 H24 Cd2 Cl4 O10
Mr	911.11	911.12
Dx,g cm ⁻³	1.827	1.827
Z	2	2
Mu (mm ⁻¹)	1.661	1.661
F000	896.0	896.0
F000'	894.33	
h,k,lmax	9,33,10	9,33,10
Nref	3431	3242
Tmin,Tmax	0.665,0.742	0.710,0.740
Tmin'	0.527	

Correction method= # Reported T Limits: Tmin=0.710 Tmax=0.740
AbsCorr = NUMERICAL

Data completeness= 0.945

Theta(max)= 26.480

R(reflections)= 0.0560(2485)

wR2(reflections)= 0.1110(2485)

S = 1.000

Npar= 208

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**

<u>PLAT029 ALERT 3 C</u>	_diffrn_measured_fraction_theta_full Low	0.960	Note
<u>PLAT342 ALERT 3 C</u>	Low Bond Precision on C-C Bonds	0.0103	Ang.
<u>PLAT758 ALERT 4 C</u>	D-H..A Calc 126.00, Rep 126.18(17)		Senseless su
	05 -H51 -O3 1.555 1.555 1.555 #	72	
<u>PLAT911 ALERT 3 C</u>	Missing # FCF Refl Between THmin & STh/L=	0.600	67 Report

● **Alert level G**

<u>PLAT007 ALERT 5 G</u>	Number of Unrefined Donor-H Atoms	1	Report
<u>PLAT128 ALERT 4 G</u>	Alternate Setting for Input Space Group P21/a	P21/c	Note
<u>PLAT152 ALERT 1 G</u>	The Supplied and Calc. Volume s.u. Differ by ...	16	Units
<u>PLAT808 ALERT 5 G</u>	No Parseable SHELXL Style Weighting Scheme Found		Please Check
<u>PLAT910 ALERT 3 G</u>	Missing # of FCF Reflection(s) Below Th(Min) ...	4	Report
<u>PLAT912 ALERT 4 G</u>	Missing # of FCF Reflections Above STh/L=	0.600	122 Note
<u>PLAT929 ALERT 5 G</u>	No Weight Pars,Obs and Calc R1,wR2,S not checked		! Info
<u>PLAT940 ALERT 3 G</u>	F**2 Refinement with I < n * Sigma(I) only		Please Check
<u>PLAT960 ALERT 3 G</u>	Number of Intensities with I < - 2*sig(I) ...		2 Check

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 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 29/01/2015; check.def file version of 29/01/2015

