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 = 0.0039 A Wavelength=0.71073

Cell: a=11.0090(9) b=10.2998(8) c=17.0078(14)
alpha=90 beta=107.988(1) gamma=90
Temperature: 295 K

	Calculated	Reported
Volume	1834.3(3)	1834.26(15)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	?
Moiety formula	C34 H26 Cd2 Cl2 N8 O10	C34 H26 Cd2 Cl2 N8 O10
Sum formula	C34 H26 Cd2 Cl2 N8 O10	C34 H26 Cd2 Cl2 N8 O10
Mr	1002.35	1002.33
Dx,g cm-3	1.815	1.815
Z	2	2
Mu (mm-1)	1.374	1.374
F000	992.0	992.0
F000’	989.76	
h,k,lmax	17,16,26	17,16,25
Nref	7622	7117
Tmin,Tmax	0.669,0.729	0.710,0.730
Tmin’	0.556	

Correction method= # Reported T Limits: Tmin=0.710 Tmax=0.730
AbsCorr = NUMERICAL

Data completeness= 0.934 Theta(max)= 34.222

R(reflections)= 0.0302(4151) wR2(reflections)= 0.0479(4151)

S = 1.000 Npar= 253

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.34	Report
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	O3	Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	N4	Check
PLAT758_ALERT_4_C	D-H..A Calc 137.00, Rep 136.85(7)	Senseless	su
	C17 -H171 -O1 1.555 1.555 1.555 # 83		
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	14	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	5	Note

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	15	Units
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cd1 -- O1 ..	6.2	su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cd1 -- O3 ..	15.0	su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cd1 -- O2_a ..	8.2	su
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please	Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Th(Min) ...	1	Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1874	Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not checked	!	Info
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	61	Check

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
2 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

Datablock 1 - ellipsoid plot