

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

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Bond precision: C-C = 0.0106 A

Wavelength=0.71073

Cell: a=9.8110(8) b=11.1289(10) c=11.4771(11)  
alpha=101.358(5) beta=90.319(5) gamma=104.641(5)  
Temperature: 295 K

	Calculated	Reported
Volume	1186.67(19)	1186.67(11)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	C52 H32 Cd2 Cl4 N4 O8	C52 H32 Cd2 Cl4 N4 O8
Sum formula	C52 H32 Cd2 Cl4 N4 O8	C52 H32 Cd2 Cl4 N4 O8
Mr	1207.44	1207.46
Dx,g cm-3	1.690	1.690
Z	1	1
Mu (mm-1)	1.182	1.182
F000	600.0	600.0
F000'	599.20	
h,k,lmax	12,13,14	12,13,14
Nref	4920	4885
Tmin,Tmax	0.785,0.854	0.820,0.850
Tmin'	0.710	

Correction method= # Reported T Limits: Tmin=0.820 Tmax=0.850  
AbsCorr = NUMERICAL

Data completeness= 0.993

Theta(max)= 26.509

R(reflections)= 0.0488( 3334)

wR2(reflections)= 0.1060( 3334)

S = 0.999

Npar= 316

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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.

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**Alert level C**

<u>PLAT094 ALERT 2 C</u>	Ratio of Maximum / Minimum Residual Density ...	2.07	Report
<u>PLAT342 ALERT 3 C</u>	Low Bond Precision on C-C Bonds .....	0.0106	Ang.
<u>PLAT911 ALERT 3 C</u>	Missing # FCF Refl Between THmin & STh/L= 0.600		8 Report

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**Alert level G**

<u>PLAT152 ALERT 1 G</u>	The Supplied and Calc. Volume s.u. Differ by ...		8 Units
<u>PLAT154 ALERT 1 G</u>	The su's on the Cell Angles are Equal .....	0.00500	Degree
<u>PLAT232 ALERT 2 G</u>	Hirshfeld Test Diff (M-X) Cd1 -- O3 ..	5.5	su
<u>PLAT232 ALERT 2 G</u>	Hirshfeld Test Diff (M-X) Cd1 -- N2 ..	6.3	su
<u>PLAT808 ALERT 5 G</u>	No Parseable SHELXL Style Weighting Scheme Found		Please Check
<u>PLAT912 ALERT 4 G</u>	Missing # of FCF Reflections Above STh/L= 0.600		28 Note
<u>PLAT929 ALERT 5 G</u>	No Weight Pars,Obs and Calc R1,wR2,S not checked		! Info
<u>PLAT960 ALERT 3 G</u>	Number of Intensities with I < - 2*sig(I) ...		6 Check

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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  
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
8 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
2 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*, 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

