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 = 0.0058 A Wavelength=0.71073 Cell: a=10.0451(3) b=10.5314(3)c=11.7004(4)alpha=100.716(2) beta=98.412(2) qamma = 109.520(1)295 K Temperature: Calculated Reported Volume 1116.88(6) 1116.88(4) P -1 Space group P -1 Hall group -P 1 Moiety formula C48 H32 Cd2 Cl4 N4 O8 C48 H32 Cd2 Cl4 N4 O8 Sum formula C48 H32 Cd2 Cl4 N4 O8 C48 H32 Cd2 Cl4 N4 O8 Mr 1159.40 1159.41 1.724 1.724 Dx,g cm-3 Ζ 1 1 Mu (mm-1)1.252 1.252 F000 576.0 576.0 F000′ 575.19 h,k,lmax 13,14,16 13,14,16 Nref 6342 6163 0.720,0.798 0.750,0.800 Tmin,Tmax Tmin' 0.706 Correction method= # Reported T Limits: Tmin=0.750 Tmax=0.800 AbsCorr = NUMERICAL Data completeness= 0.972 Theta(max) = 29.694 R(reflections) = 0.0371(4917) wR2(reflections) = 0.0626(4917) S = 1.000Npar= 316

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
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite
                                                                          5 Note
                                                                         5 Report
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
                                                                         2 Units
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cd1 -- O3_a ..
                                                                       5.5 su
<u>PLAT300_ALERT_4_G</u> Atom Site Occupancy of *04 is Constrained at 0.500 Check 
<u>PLAT300_ALERT_4_G</u> Atom Site Occupancy of *05 is Constrained at 0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C14 is Constrained at
                                                                     0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C25 is Constrained at
                                                                     0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *04_a is Constrained at
                                                                     0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *O5_a is Constrained at
                                                                     0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C14_a is Constrained at
                                                                    0.500 Check
PLAT300_ALERT_4_G Atom Site Occupancy of *C25_a is Constrained at
                                                                     0.500 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage =
                                                                          6 Note
PLAT431_ALERT_2_G Short Inter HL..A Contact Cl2 .. 05 ...
                                                                      3.12 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #
                                                                        53 Check
             C14 -C8 -C25 1.555 1.555 1.555
                                                                   18.00 Deg.
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found
                                                                   Please Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
                                                                         30 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
                                                                       178 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) ...
                                                                        224 Check
```

```
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
- 20 ALERT level G = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 4 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
- 10 ALERT type 4 Improvement, methodology, query or suggestion
- 2 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

