

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_sq

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_sq

Bond precision: C-C = 0.0040 A

Wavelength=0.71073

Cell: a=10.396(3) b=15.684(4) c=16.552(4)
 alpha=115.720(8) beta=99.619(10) gamma=96.034(10)
Temperature: 273 K

	Calculated	Reported
Volume	2348.8(11)	2348.7(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C27 H40 Ca N12 O11), C6 H5 N O3, 2(Cd Cl4) [+ solvent]	2(Cd Cl4), C54 H80 Ca2 N24 O22, 0.5(C12 H10 N2 O6)
Sum formula	C60 H85 Ca2 Cd2 Cl8 N25 O25 [+ solvent]	C60 H85 Ca2 Cd2 Cl8 N25 O25
Mr	2145.11	2145.08
Dx, g cm ⁻³	1.517	1.517
Z	1	1
Mu (mm ⁻¹)	0.869	0.869
F000	1092.0	1092.0
F000'	1092.45	
h,k,lmax	13,20,22	13,20,22
Nref	11682	11588
Tmin,Tmax		0.564,0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.564 Tmax=0.746
AbsCorr = NONE

Data completeness= 0.992

Theta(max)= 28.314

R(reflections)= 0.0533(9470)

wR2(reflections)= 0.1680(11588)

S = 1.034

Npar= 620

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

PLAT420_ALERT_2_B D-H Without Acceptor 011 --H11 . Please Check

Alert level C

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Ca1 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C12 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.8 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including 09 0.107 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cd1A 0.102 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 34 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 7 Note
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 11 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 273 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 273 Check
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Cd1A --C12 . 6.4 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Cd1A --C13 . 6.4 s.u.
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent) Cd1 --C11 . 10.6 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O9 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O10 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O11 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N13 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C27 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C28 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C29 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C30 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H27 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H28 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H30 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31 Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 90% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 60% Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 128 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 3 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 14 Check
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 55 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 9 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
33 **ALERT level G** = General information/check it is not something unexpected

7 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
25 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* or *IUCrData*, 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 18/09/2020; check.def file version of 20/08/2020

