

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cp1-3, cp1-4, cp1-5

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: cp1-3

Bond precision: C-C = 0.0113 Å Wavelength=1.34138

Cell: a=14.8801 (12) b=33.650 (3) c=28.297 (3)
 alpha=90 beta=103.897 (3) gamma=90

Temperature: 273 K

	Calculated	Reported
Volume	13754 (2)	13754 (2)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	2 (C35 H24 Cd Cl4 N2 O5)
Sum formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	C70 H48 Cd2 Cl8 N4 O10
Mr	1613.55	1613.52
Dx, g cm ⁻³	1.559	1.558
Z	8	8
Mu (mm ⁻¹)	5.608	5.608
F000	6464.0	6464.0
F000'	6498.35	
h, k, lmax	17, 40, 33	17, 40, 33
Nref	24325	24237
Tmin, Tmax	0.670, 0.755	0.431, 0.752
Tmin'	0.608	

Correction method= # Reported T Limits: Tmin=0.431 Tmax=0.752
AbsCorr = NONE

Data completeness= 0.996 Theta (max)= 52.981

R(reflections)= 0.0724(18408)

wR2(reflections)=
0.2144(24237)

S = 1.028

Npar= 1779

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 Bond Without Acceptor	O17	--H17A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O18	--H18	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O19	--H19A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O20	--H20	.	Please Check



Alert level C

PLAT057_ALERT_3_C	Correction for Absorption Required	RT(exp) ...	1.13	Do !
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C Ueq(max)/Ueq(min) Range	3.4	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 1 O Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1 H Uiso(max)/Uiso(min) Range	5.1	Ratio
PLAT223_ALERT_4_C	Solv./Anion	Resd 2 H Ueq(max)/Ueq(min) Range	4.1	Ratio
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	01	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	02	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	03	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	04	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	05	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	08	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C16	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C18	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	O10	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	O11	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	O12	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	O13	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C32	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C40	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C97	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C98	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Cd1	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Cd2	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C8	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C15	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C17	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C20	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C112	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C131	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Cd3	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Cd4	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N4	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C31	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C33	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C35	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C39	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C41	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C46	Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C94 Check
 PLAT329_ALERT_4_C Carbon Atom Hybridisation Unclear for C2 Check
 PLAT334_ALERT_2_C Small <C-C> Benzene Dist. C8 -C13 . 1.37 Ang.
 PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01126 Ang.
 PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C15 - C16 . 1.53 Ang.
 PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C50 - C51 . 1.53 Ang.
 PLAT414_ALERT_2_C Short Intra D-H..H-X H18 ..H128 . 1.96 Ang.
 x,y,z = 1_555 Check
 PLAT414_ALERT_2_C Short Intra D-H..H-X H19A ..H66B . 1.92 Ang.
 x,y,z = 1_555 Check
 PLAT414_ALERT_2_C Short Intra D-H..H-X H20 ..H90 . 1.98 Ang.
 x,y,z = 1_555 Check
 PLAT415_ALERT_2_C Short Inter D-H..H-X H19A ..H71 . 2.11 Ang.
 2-x,-y,1-z = 3_756 Check
 PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 4.181 Check
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 87 Report
 4 0 0, 7 1 0, 0 4 0, 2 8 0, 0 12 0, -1 2 1,
 1 2 1, 3 2 1, 7 2 1, -4 3 1, 0 7 1, 3 10 1,
 0 0 2, 4 0 2, -7 1 2, -3 1 2, 3 1 2, -4 2 2,
 4 2 2, -1 3 2, 0 4 2, 2 4 2, 6 4 2, -1 7 2,
 0 8 2, -1 9 2, 0 1 3, -1 2 3, 3 2 3, 7 2 3,
 -8 3 3, -4 3 3, -2 3 3, 0 3 3, 0 5 3, -1 6 3,
 -1 8 3, -4 11 3, -7 33 3, -6 0 4, 0 0 4, 6 0 4,
 -1 1 4, 3 1 4, 0 4 4, 2 4 4, -3 5 4, -1 5 4,
 3 5 4, -1 7 4, 0 8 4, -1 9 4, -1 13 4, -8 27 4,
 0 3 5, -1 6 5, -1 8 5, -1 9 5, -2 0 6, 1 1 6,
 -2 2 6, -1 5 6, -1 9 6, -1 13 6, -1 2 7, -5 6 7,
 -1 6 7, 3 29 7, 6 27 8, -1 2 9, -1 10 9, 2 0 10,
 -2 4 10, 2 27 10, 2 26 11, 1 26 12, 1 28 12, 1 25 13,
 0 2 14, 7 1 20, 0 18 21, 4 0 22, 3 6 23, -4 1 25,
 -4 2 25, -4 3 25, -4 11 25,
 PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 18 Note
 4 0 0, 7 2 1, 0 0 2, 4 0 2, -4 2 2, 0 4 2,
 -1 7 2, 0 8 2, 3 2 3, 7 2 3, 0 3 3, -1 8 3,
 -1 5 4, -1 9 4, -1 9 5, -1 5 6, -1 9 6, -1 13 6,
 PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
 PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.56Ang From O19 . -0.67 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H11B . -0.40 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H13A . -0.33 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H18 . -0.42 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H19A . -0.40 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H20 . -0.40 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H21 . -0.38 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
 not performed for this radiation type.
 PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 28 Note
 PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms 200 Report
 PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
 H17A H18 H19A H20
 PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 Calc: C70 H48 Cd2 Cl8 N4 O10
 Rep.: 2(C35 H24 Cd Cl4 N2 O5)
 PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	49.69	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		14	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		8	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		4	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for SecondPar		0.0200	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K)	273	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	(K)	273	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	13%	Note
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C16	-C21	0.16	Ang.
PLAT410_ALERT_2_G	Short Intra H...H Contact H2A	..H138	2.11	Ang.
		x,y,z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H3A	..H100	2.07	Ang.
		x,y,z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H138	..H2	1.91	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C110	..C20	3.24	Ang.
		1-x,-1/2+y,3/2-z =	2_646	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact C17	..C112	3.31	Ang.
		x,1/2-y,-1/2+z =	4_565	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		167	A**3
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C133	--C2	1.85	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C136	--C1	1.74	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C1	--C4	1.71	Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd2	(II)	1.96	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd3	(II)	2.04	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cd4	(II)	2.05	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		694	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed		!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary		Please	Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		49%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
	0 1 1,			
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		5	Note
	-3 1 2, 0 0 4, 0 1 1, 0 2 14, 4 2 2,			
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		4.442	Note
	Predicted wR2: Based on SigI**2 4.83 or SHELX Weight 20.87			
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 69 ALERT type 2 Indicator that the structure model may be wrong or deficient
 17 ALERT type 3 Indicator that the structure quality may be low
 8 ALERT type 4 Improvement, methodology, query or suggestion
 6 ALERT type 5 Informative message, check

Datablock: cp1-4

Bond precision: C-C = 0.0122 Å Wavelength=1.34138

Cell: a=14.893(4) b=33.653(10) c=28.302(8)
alpha=90 beta=104.480(11) gamma=90

Temperature: 273 K

	Calculated	Reported
Volume	13734(7)	13734(7)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	2(C35 H24 Cd Cl4 N2 O5)
Sum formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	C70 H48 Cd2 Cl8 N4 O10
Mr	1613.55	1613.52
Dx, g cm ⁻³	1.561	1.561
Z	8	8
Mu (mm ⁻¹)	5.616	5.616
F000	6464.0	6464.0
F000'	6498.35	
h, k, lmax	17, 40, 33	17, 40, 33
Nref	24278	24104
Tmin, Tmax	0.599, 0.638	0.480, 0.685
Tmin'	0.543	

Correction method= # Reported T Limits: Tmin=0.480 Tmax=0.685
AbsCorr = NONE

Data completeness= 0.993 Theta(max)= 52.979

R(reflections)= 0.1016(18517) wR2(reflections)=
0.3113(24104)

S = 1.075 Npar= 1696

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 Bond Without Acceptor	O17	--H17A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O18	--H18	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O19	--H19A	.	Please Check

PLAT420_ALERT_2_B D-H Bond Without Acceptor O20 --H20 . Please Check



Alert level C

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.31	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.49	Report
PLAT213_ALERT_2_C	Atom Cl3A has ADP max/min Ratio	3.5	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.2	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 2 H Uiso(max)/Uiso(min) Range	4.2	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	010	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	015	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	02	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	05	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C4	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C6	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C11	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C13	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C18	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C65	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C98	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Cd1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Cd2	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C45	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C46	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C47	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C55	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C109	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C127	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including Cd3	0.109	Check
PLAT329_ALERT_4_C	Carbon Atom Hybridisation Unclear for	C63A	Check
PLAT329_ALERT_4_C	Carbon Atom Hybridisation Unclear for	C83A	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01218	Ang.
PLAT361_ALERT_2_C	Long C(sp3)-C(sp3) Bond C105 - C126 .	1.66	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C36 - C37 .	1.54	Ang.
PLAT414_ALERT_2_C	Short Intra D-H..H-X H20 ..H87 .	1.99	Ang.
	x,y,z =	1_555	Check
PLAT702_ALERT_1_C	Angle Calc 85.6(3), Rep 86(2), Dev..	1.33	Sigma
	N3 -CD4 -C1 2_545 1_555 1_555 #	84	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.895	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.008	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595	173 Report
	4 0 0, 14 1 0, 15 2 0, 10 3 0, 0 4 0, 11 1 1,		
	-1 2 1, -11 3 1, -14 4 1, 1 4 1, 8 4 1, 13 7 1,		
	-12 8 1, -4 39 1, -3 0 2, 0 0 2, 10 1 2, 14 1 2,		
	-15 2 2, -4 2 2, -1 3 2, 14 3 2, 0 4 2, -15 6 2,		
	-8 7 2, -1 7 2, 0 8 2, -4 39 2, 0 1 3, -1 2 3,		
	3 2 3, 0 3 3, -14 4 3, 0 5 3, 2 5 3, 13 5 3,		
	11 7 3, -1 8 3, -4 39 3, 13 2 4, 0 4 4, -1 5 4,		
	11 8 4, -1 9 4, -15 1 5, -13 3 5, 13 3 5, 6 4 5,		
	10 4 5, 11 7 5, 5 2 6, 7 2 6, 9 2 6, 13 2 6,		
	4 3 6, -3 5 6, -1 5 6, 7 6 6, -1 9 6, -15 1 7,		
	3 1 7, 5 1 7, -15 3 7, 3 3 7, 5 3 7, 6 4 7,		
	10 4 7, -13 5 7, 10 8 7, 6 1 8, 2 3 8, 6 3 8,		
	10 3 8, -12 9 8, -5 11 8, -2 11 8, 5 1 9, 5 3 9,		
	2 4 9, -1 5 9, 5 7 9, 3 9 9, 5 9 9, 9 11 9,		
	2 1 10, 6 1 10, 10 1 10, 1 2 10, 3 2 10, 4 3 10,		

PLAT415_ALERT_2_G Short Inter D-H...H-X H20 ..H63A . 2.10 Ang.
 $-x, 1-y, -z = 3_565$ Check
 PLAT432_ALERT_2_G Short Inter X...Y Contact Cl7 ..C41 . 3.16 Ang.
 $1-x, 1/2+y, 1/2-z = 2_655$ Check
 PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl4 ..Cl11 . 3.36 Ang.
 $x, 3/2-y, 1/2+z = 4_576$ Check
 PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl5 ..Cl14 . 3.22 Ang.
 $x, 3/2-y, -1/2+z = 4_575$ Check
 PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 119 A**3
 PLAT773_ALERT_2_G Check long C-C Bond in CIF: C81 --C83A 1.77 Ang.
 PLAT773_ALERT_2_G Check long C-C Bond in CIF: C67 --C63A 1.85 Ang.
 PLAT794_ALERT_5_G Tentative Bond Valency for Cd1 (II) . 1.93 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Cd2 (II) . 2.03 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Cd3 (II) . 2.06 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Cd4 (II) . 2.04 Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 3412 Note
 PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info
 PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
 PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 43% Note
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
 0 1 1,
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 12 Note
 -5 11 8, -3 0 2, -3 5 6, -1 5 4, -1 5 6, -1 9 6,
 0 1 1, 0 3 3, 0 5 3, 1 4 1, 2 5 3, 3 2 3,
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 6.270 Note
 Predicted wR2: Based on SigI**2 4.96 or SHELX Weight 28.94
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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 8 ALERT type 4 Improvement, methodology, query or suggestion
 7 ALERT type 5 Informative message, check

Datablock: cp1-5

Bond precision: C-C = 0.0097 A Wavelength=1.34138

Cell: a=14.9038(18) b=33.566(4) c=28.295(3)
 alpha=90 beta=104.988(4) gamma=90

Temperature: 273 K

	Calculated	Reported
Volume	13673(3)	13673(3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	2(C35 H24 Cd Cl4 N2 O5)
Sum formula	C70 H48 Cd2 Cl8 N4 O10 [+ solvent]	C70 H48 Cd2 Cl8 N4 O10
Mr	1613.55	1613.52
Dx, g cm ⁻³	1.568	1.568
Z	8	8
Mu (mm ⁻¹)	5.641	5.641
F000	6464.0	6464.0
F000'	6498.35	
h, k, lmax	17, 40, 33	17, 39, 33
Nref	24425	24185
Tmin, Tmax	0.669, 0.754	0.484, 0.751
Tmin'	0.606	

Correction method= # Reported T Limits: Tmin=0.484 Tmax=0.751
AbsCorr = NONE

Data completeness= 0.990 Theta(max)= 53.258

R(reflections)= 0.0971(18147) wR2(reflections)=
0.3291(24185)

S = 1.069 Npar= 1484

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 Bond Without Acceptor	O17	--H17	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O18A	--H18A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O19	--H19	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O20	--H20	.	Please Check
PLAT973_ALERT_2_B	Check Calcd Positive Resid. Density on			Cd3	1.94 eA-3

Alert level C

PLAT057_ALERT_3_C	Correction for Absorption Required	RT(exp) ...	1.13	Do !
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)		0.33	Report
PLAT213_ALERT_2_C	Atom Cl3	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom Cl6	has ADP max/min Ratio	3.3	prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1 Cl Ueq(max)/Ueq(min) Range	3.1	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 1 O Ueq(max)/Ueq(min) Range	4.7	Ratio

PLAT222_ALERT_3_C	NonSolvent Resd 1	H	Uiso(max)/Uiso(min) Range	6.4	Ratio													
PLAT222_ALERT_3_C	NonSolvent Resd 2	H	Uiso(max)/Uiso(min) Range	4.2	Ratio													
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	01	Check													
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	02	Check													
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	05	Check													
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	013	Check													
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	015	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Cd1	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Cd2	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C20	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C99	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C100	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C101	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C102	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C106	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C107	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C109	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Cd4	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C59	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C71	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C113	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C115	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C130	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C132	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C138	Check													
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C140	Check													
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		Cd3	0.102	Check													
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds		0.00969	Ang.													
PLAT361_ALERT_2_C	Long	C(sp3)-C(sp3) Bond	C31 - C32 .	1.67	Ang.													
PLAT363_ALERT_2_C	Long	C(sp3)-C(sp2) Bond	C47 - C53 .	1.64	Ang.													
PLAT363_ALERT_2_C	Long	C(sp3)-C(sp2) Bond	C52 - C54 .	1.67	Ang.													
PLAT368_ALERT_2_C	Short	C(sp2)-C(sp2) Bond	C99 - C100 .	1.21	Ang.													
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond	C76 - C78 .	1.54	Ang.													
PLAT410_ALERT_2_C	Short	Intra H...H Contact	H30 ..H39 .	1.92	Ang.													
			x,y,z =	1_555	Check													
PLAT414_ALERT_2_C	Short	Intra D-H...H-X	H17 ..H20A .	1.98	Ang.													
			x,y,z =	1_555	Check													
PLAT414_ALERT_2_C	Short	Intra D-H...H-X	H19 ..H71B .	1.99	Ang.													
			x,y,z =	1_555	Check													
PLAT415_ALERT_2_C	Short	Inter D-H...H-X	H20 ..H56 .	2.12	Ang.													
			2-x,-y,1-z =	3_756	Check													
PLAT731_ALERT_1_C	Bond	Calc	2.380(5), Rep	2.38(3)	6 su-Rat													
	CD2	-N2	1_555	2_645	# 7 Check													
PLAT731_ALERT_1_C	Bond	Calc	2.295(4), Rep	2.295(16)	4 su-Rat													
	CD3	-N5	1_555	2_755	# 14 Check													
PLAT731_ALERT_1_C	Bond	Calc	2.335(3), Rep	2.335(11)	4 su-Rat													
	CD1	-N1	1_555	2_645	# 20 Check													
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			3.905	Check													
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.597		231	Report													
	2	0	0,	4	0	0,	0	4	0,	17	6	0,	2	8	0,	0	12	0,
	4	39	0,	4	1	1,	-1	2	1,	3	2	1,	-4	3	1,	17	3	1,
	3	10	1,	15	19	1,	-15	20	1,	-12	29	1,	-11	31	1,	-4	39	1,
	0	0	2,	4	0	2,	-7	1	2,	-3	1	2,	-1	1	2,	-4	2	2,
	-1	3	2,	0	4	2,	2	4	2,	-1	7	2,	0	8	2,	-17	9	2,
	-1	9	2,	5	9	2,	-16	16	2,	-14	24	2,	10	32	2,	8	35	2,
	5	38	2,	-4	39	2,	-4	1	3,	0	1	3,	-1	2	3,	3	2	3,
	7	2	3,	-2	3	3,	0	3	3,	0	5	3,	-1	8	3,	-4	11	3,

-13 27 3, -10 33 3, 7 36 3, 6 37 3, -4 39 3, -14 0 4,	
6 0 4, -1 1 4, 0 4 4, -5 5 4, -1 5 4, -1 7 4,	
1 7 4, -1 9 4, 12 27 4, 9 33 4, 0 3 5, 2 3 5,	
-1 6 5, 2 7 5, -17 11 5, -4 11 5, 14 20 5, 8 34 5,	
4 38 5, -2 0 6, 2 0 6, 1 1 6, -2 2 6, 16 4 6,	
-1 5 6, -1 9 6, 3 9 6, -1 13 6, 15 14 6, 14 19 6,	
9 32 6, 7 35 6, 6 36 6, 5 37 6, -3 39 6, 2 3 7,	
2 5 7, -1 6 7, 2 7 7, 12 25 7, -10 33 7, -5 38 7,	
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF	23 Note
4 0 0, 0 4 0, 3 2 1, -4 3 1, 0 0 2, -7 1 2,	
-4 2 2, 0 4 2, -1 7 2, 0 8 2, -4 1 3, 3 2 3,	
7 2 3, 0 3 3, -1 8 3, -4 11 3, 0 4 4, -5 5 4,	
-1 5 4, -1 9 4, -1 5 6, -1 9 6, -1 13 6,	
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .	17 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.29Ang From Cd2	2.22 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.75Ang From Cd4	1.76 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.19Ang From C54	1.62 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.72Ang From C99	1.53 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.20Ang From C74	1.52 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.47Ang From Cl15	1.52 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H17 .	-0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H88 .	-0.31 eA-3

● Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	15 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms	143 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms	5 Report
H17 H18A H18B H19 H20	
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ	Please Check
Calc: C70 H48 Cd2 Cl8 N4 O10	
Rep.: 2(C35 H24 Cd Cl4 N2 O5)	
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large	0.22 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	30.12 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	9 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records	4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records	7 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used	0.0100 Report
PLAT191_ALERT_3_G A Non-default SADI Restraint Value has been used	0.0400 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K)	273 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K)	273 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1)	2% Note
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C99 -C101	0.26 Ang.
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for	C55 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for	C56 Check
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C53 - C56 .	1.54 Ang.
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C54 - C55 .	1.51 Ang.
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C56 - C74 .	1.61 Ang.
PLAT411_ALERT_2_G Short Inter H...H Contact H59B ..H23C .	1.95 Ang.
x,1/2-y,1/2+z =	4_566 Check
PLAT415_ALERT_2_G Short Inter D-H...H-X H3 ..H18A .	2.03 Ang.
1-x,1-y,-z =	3_665 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl9 ..C85 .	3.20 Ang.

	1-x,1/2+y,1/2-z =	2_655 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C59 ..C23A .	3.20 Ang.
	x,1/2-y,1/2+z =	4_566 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact	C15 ..C116 .	3.26 Ang.
	x,1/2-y,1/2+z =	4_566 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact	C18 ..C111 .	3.22 Ang.
	x,1/2-y,-1/2+z =	4_565 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure		137 A**3
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C55	--C56	1.80 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1	(II) .	2.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd2	(II) .	1.95 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd3	(II) .	2.11 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cd4	(II) .	2.03 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints		3234 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed		! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still		42% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File		2 Note
	1 7 4, 5 9 2,	
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value		7.182 Note
	Predicted wR2: Based on SigI**2 4.58 or SHELX Weight 30.79	
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		0 Info

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

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 70 ALERT type 2 Indicator that the structure model may be wrong or deficient
 14 ALERT type 3 Indicator that the structure quality may be low
 6 ALERT type 4 Improvement, methodology, query or suggestion
 7 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.





