

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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 = 0.0127 Å	Wavelength=0.71073	
Cell:	a=37.342(7)	b=8.2819(4)	c=26.577(9)
	alpha=90	beta=134.36(3)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	5877(4)	5877(2)	
Space group	C 2/c	C2/c	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C60 H38 N12 O14 Zn3, 4(H2 O)	?	
Sum formula	C60 H46 N12 O18 Zn3	C60 H46 N12 O18 Zn3	
Mr	1419.26	1419.26	
Dx, g cm ⁻³	1.604	1.604	
Z	4	4	
Mu (mm ⁻¹)	1.301	1.301	
F000	2896.0	2896.0	
F000'	2900.63		
h, k, lmax	44, 9, 31	44, 9, 31	
Nref	5166	5160	
Tmin, Tmax	0.855, 0.901	0.855, 0.901	
Tmin'	0.812		

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 25.000

R(reflections)= 0.0794(3093) wR2(reflections)= 0.1575(5160)

S = 1.043 Npar= 421

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 09 - H9B ... Please Check

🟢 Alert level C

PLAT048_ALERT_1_C MoietyFormula Not Given Please Do !
PLAT234_ALERT_4_C Large Hirshfeld Difference N6 -- C14 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22 -- C23 .. 0.18 Ang.
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for 05 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C1 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C2 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C13 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C26 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for N5 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for N6 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C24 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C29 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C30 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0127 Ang.
PLAT417_ALERT_2_C Short Inter D-H..H-D H8A .. H9A .. 2.13 Ang.

🟠 Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 13 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension 3 Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Why ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 19.21
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as . mixed
PLAT128_ALERT_4_G Alternate Setting for Input Space-Group C2/c I2/a Note
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 2 Units
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT230_ALERT_2_G Hirshfeld Test Diff for N5 -- C15A .. 9.1 su
PLAT230_ALERT_2_G Hirshfeld Test Diff for N6 -- C14A .. 11.1 su
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Zn2 -- O4_j .. 24.5 su
PLAT301_ALERT_3_G Main Residue Disorder Percentage = 4 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.13 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 114
C15 -N5 -C15A 1.555 1.555 1.555 39.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 120
C14 -N6 -C14A 1.555 1.555 1.555 38.30 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3
H2 O
PLAT860_ALERT_3_G Number of Least-Squares Restraints 18 Note

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
17 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
7 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

Datablock: 2

Bond precision: C-C = 0.0096 Å

Wavelength=0.71073

Cell: a=38.1051(19) b=8.0262(2) c=26.1036(12)
alpha=90 beta=130.755(8) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	6047.6(8)	6047.6(4)
Space group	C 2/c	C2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C60 H42 Cd3 N12 O16, 6(H2 O)	?
Sum formula	C60 H54 Cd3 N12 O22	C60 H54 Cd3 N12 O22
Mr	1632.38	1632.38
Dx, g cm ⁻³	1.793	1.793
Z	4	4
Mu (mm ⁻¹)	1.139	1.139
F000	3272.0	3272.0
F000'	3263.84	
h, k, lmax	45, 9, 31	45, 9, 31
Nref	5342	5335
Tmin, Tmax	0.815, 0.872	0.815, 0.872
Tmin'	0.796	

Correction method= MULTI-SCAN

Data completeness= 0.999

Theta(max)= 25.000

R(reflections)= 0.0531(4048)

wR2(reflections)= 0.1049(5335)

S = 1.084

Npar= 438

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 A

PLAT415_ALERT_2_A Short Inter D-H..H-X	H9	..	H10A	..	1.79 Ang.
PLAT417_ALERT_2_A Short Inter D-H..H-D	H8A	..	H11A	..	1.73 Ang.

Alert level B

PLAT220_ALERT_2_B Large Non-Solvent	0	Ueq(max)/Ueq(min)	...	4.8 Ratio
PLAT417_ALERT_2_B Short Inter D-H..H-D	H10B	..	H11B	.. 1.94 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor	O10	-	H10B	... Please Check

Alert level C

PLAT048_ALERT_1_C MoietyFormula Not Given		Please Do !
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PLAT213_ALERT_2_C	Atom O3	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C23	has ADP max/min Ratio	3.8	prolat
PLAT222_ALERT_3_C	Large Non-Solvent H	Uiso(max)/Uiso(min) ..	5.4	Ratio
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	07	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	Cd2	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C23	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0096	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C22 - C23 ...		1.53	Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	12	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1	
PLAT004_ALERT_5_G	Polymeric Structure Found with Dimension	3	Info
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF		Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	8	Why ?
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	45.78	
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as .	mixed	
PLAT128_ALERT_4_G	Alternate Setting for Input Space-Group C2/c	I2/a	Note
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	4	Units
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	293	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	18	Note

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5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 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
 3 ALERT type 5 Informative message, check

Datablock: 3

Bond precision:	C-C = 0.0163 A	Wavelength=0.71073
Cell:	a=10.1513(15)	b=32.003(6) c=18.417(4)
	alpha=90	beta=90 gamma=90
Temperature:	293 K	

	Calculated	Reported
Volume	5983.2(19)	5983.3(19)
Space group	P c c n	P c c n
Hall group	-P 2ab 2ac	-P 2ab 2ac
Moiety formula	C60 H38 N12 O14 Zn3, O	?
Sum formula	C60 H38 N12 O15 Zn3	C60 H38 N12 O15 Zn3
Mr	1363.19	1363.19
Dx, g cm ⁻³	1.513	1.513
Z	4	4
Mu (mm ⁻¹)	1.271	1.271
F000	2768.0	2768.0
F000'	2772.52	
h, k, l _{max}	12, 38, 21	12, 38, 21
Nref	5261	5244
Tmin, Tmax	0.808, 0.881	0.808, 0.881
Tmin'	0.806	

Correction method= MULTI-SCAN

Data completeness= 0.997

Theta(max)= 25.000

R(reflections)= 0.0987(2377)

wR2(reflections)= 0.3063(5244)

S = 0.952

Npar= 407

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

PLAT234_ALERT_4_B	Large Hirshfeld Difference 07	-- C15 ..	0.28 Ang.
PLAT242_ALERT_2_B	Low	Ueq as Compared to Neighbors for	C15 Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)		08 Check
PLAT341_ALERT_3_B	Low Bond Precision on C-C Bonds		0.0163 Ang.
PLAT369_ALERT_2_B	Long C(sp ²)-C(sp ²) Bond C14 - C15 ...		1.62 Ang.

🟡 Alert level C

RFACR01_ALERT_3_C	The value of the weighted R factor is > 0.25	
	Weighted R factor given	0.306
RINTA01_ALERT_3_C	The value of Rint is greater than 0.12	
	Rint given	0.136
PLAT020_ALERT_3_C	The value of Rint is greater than 0.12	0.136
PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections too Low	45 %
PLAT048_ALERT_1_C	MoietyFormula Not Given	Please Do !
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.31
PLAT234_ALERT_4_C	Large Hirshfeld Difference 01 -- C1 ..	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N3 -- C29 ..	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C3 -- C4 ..	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C3 -- C8 ..	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C6 -- C7 ..	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C13 -- C14 ..	0.21 Ang.

PLAT234_ALERT_4_C	Large Hirshfeld Difference C19 -- C20 ..	0.16 Ang.
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	03 Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	05 Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	C14 Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	C30 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	Zn1 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	N3 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	N4 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	C9 Check
PLAT334_ALERT_2_C	Small Average Benzene C-C Dist. C3 -C8	1.37 Ang.
PLAT334_ALERT_2_C	Small Average Benzene C-C Dist. C9 -C14	1.36 Ang.
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .	95 Ang3

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	3 Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Dimension	3 Info
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.17
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as .	mixed
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	293 Check
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C9 -C14	0.15 Ang.
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	5 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2 Note

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

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

Datablock: 4

Bond precision:	C-C = 0.0080 A	Wavelength=0.71073
Cell:	a=32.5833(8)	b=10.1910(3) c=19.1380(5)
	alpha=90	beta=90 gamma=90
Temperature:	293 K	

	Calculated	Reported
Volume	6354.9(3)	6354.9(3)
Space group	P c c n	P c c n
Hall group	-P 2ab 2ac	-P 2ab 2ac
Moiety formula	C60 H38 Cd3 N12 O14, 5(H2 O), O	?
Sum formula	C60 H48 Cd3 N12 O20	C60 H48 Cd3 N12 O20
Mr	1594.33	1594.33
Dx,g cm-3	1.666	1.666
Z	4	4
Mu (mm-1)	1.079	1.079
F000	3184.0	3184.0
F000'	3175.76	
h,k,lmax	38,12,22	38,12,22
Nref	5597	5584
Tmin,Tmax	0.834,0.917	0.834,0.917
Tmin'	0.823	

Correction method= MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.000

R(reflections)= 0.0459(4479) wR2(reflections)= 0.1119(5584)

S = 1.082 Npar= 434

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	09	-	*H9A	...	Please Check
PLAT420_ALERT_2_B	D-H Without Acceptor	010	-	H10A	...	Please Check
PLAT420_ALERT_2_B	D-H Without Acceptor	010	-	H10B	...	Please Check

Alert level C

PLAT048_ALERT_1_C	MoietyFormula Not Given	Please Do !
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.29
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Cd1 -- 05_d ..	7.7 su
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	01 Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	02 Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	03 Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	C15 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	Cd2 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	N5 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	C30 Check
PLAT334_ALERT_2_C	Small Average Benzene C-C Dist. C17 -C22	1.37 Ang.

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	9 Note
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PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6 Why ?
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	18.02
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as .	mixed
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293 Check
PLAT302_ALERT_4_G	Anion/Solvent Disorder Percentage =	14 Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	011 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.19 Ratio
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2
	H2 O	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3
	H2 O	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	4
	H2 O	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	5
	O	
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	31 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	9 Note

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

Datablock: 5

Bond precision: C-C = 0.0093 A

Wavelength=0.71073

Cell:	a=19.9674(5)	b=18.9868(5)	c=30.7298(11)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	11650.2(6)	11650.2(6)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	2(C60 H38 N12 O14 Zn3), 6(H 00.50), 4(O)	?
Sum formula	C120 H86 N24 O37 Zn6	C60 H43 N12 O18.50 Zn3
Mr	2848.47	1424.17
Dx, g cm-3	1.624	1.624
Z	4	8
Mu (mm-1)	1.314	1.314
F000	5800.0	5800.0
F000'	5809.31	
h, k, lmax	23, 22, 36	23, 22, 36
Nref	10258	10230
Tmin, Tmax	0.777, 0.854	0.777, 0.854
Tmin'	0.749	

Correction method= MULTI-SCAN

Data completeness= 0.997

Theta(max)= 25.000

R(reflections)= 0.0662(5960)

wR2(reflections)= 0.1866(10230)

S = 0.998

Npar= 837

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

PLAT220_ALERT_2_B	Large Non-Solvent	C	Ueq(max)/Ueq(min) ...	4.4	Ratio
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)			017	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)			019	Check
PLAT420_ALERT_2_B	D-H Without Acceptor	015	- H15A ...		Please Check
PLAT420_ALERT_2_B	D-H Without Acceptor	016	- H16A ...		Please Check
PLAT420_ALERT_2_B	D-H Without Acceptor	*018	- *H18B ...		Please Check

Alert level C

PLAT048_ALERT_1_C	MoietyFormula Not Given				Please Do !
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density			2.65	
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent			1	
PLAT222_ALERT_3_C	Large Non-Solvent	H	Uiso(max)/Uiso(min) ..	4.1	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference N5	--	C42 ..	0.19	Ang.
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for		013	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for		C28	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for		C41	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for		C42	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for		N5	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for		N6	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds			0.0093	Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	9	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2	
PLAT004_ALERT_5_G	Polymeric Structure Found with Dimension	3	Info
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please	Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6	Why ?
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by	0.50	Ratio
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as .	mixed	
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT302_ALERT_4_G	Anion/Solvent Disorder Percentage =	11	Note
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	10	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	21	Note

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4 ALERT type 5 Informative message, check

Datablock: 6

Bond precision: C-C = 0.0125 A

Wavelength=0.71073

Cell: a=7.5481(6) b=10.8878(10) c=19.0460(18)
alpha=79.948(8) beta=79.570(8) gamma=73.077(8)
Temperature: 293 K

	Calculated	Reported
Volume	1460.3(2)	1460.3(2)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C60 H40 N12 O14 Zn2, H2 O	?
Sum formula	C60 H42 N12 O15 Zn2	C60 H42 N12 O15 Zn2
Mr	1301.84	1301.80
Dx, g cm-3	1.480	1.480
Z	1	1
Mu (mm-1)	0.901	0.901
F000	666.0	666.0
F000'	666.85	
h, k, lmax	8, 12, 22	8, 12, 22
Nref	10250[5125]	8154
Tmin, Tmax	0.878, 0.914	0.878, 0.914
Tmin'	0.850	

Correction method= MULTI-SCAN

Data completeness= 1.59/0.80 Theta(max)= 25.000

R(reflections)= 0.0617(7027) wR2(reflections)= 0.1680(8154)

S = 1.049 Npar= 802

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	07	-	H7A	...	Please Check
PLAT420_ALERT_2_B	D-H Without Acceptor	015	-	H15A	...	Please Check
PLAT601_ALERT_2_B	Structure Contains Solvent Accessible VOIDS of					108 Ang3

 Alert level C

PLAT048_ALERT_1_C	MoietyFormula Not Given					Please Do !
PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)					6.39
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density					3.83
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	03	--	C2	..	5.2 su
PLAT234_ALERT_4_C	Large Hirshfeld Difference	06	--	C15	..	0.17 Ang.
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for					01 Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for					C45 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for					C1 Check
PLAT309_ALERT_2_C	Single Bonded Oxygen (C-O > 1.3 Ang)					06 Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds					0.0125 Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C17	-	C19	...	1.53 Ang.
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd.	#				1
	C60 H40 N12 O14 Zn2					

 Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					7 Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Dimension					3 Info
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF					Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms					4 Why ?
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.					0.10
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as	.				mixed
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal					0.00800 Deg.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	 (K)				293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	 (K)				293 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd.	#				2
	H2 O					
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 and su	..				0.02
PLAT860_ALERT_3_G	Number of Least-Squares Restraints					8 Note

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

3 **ALERT level B** = A potentially serious problem, consider carefully

12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

5 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data

- 12 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
 4 ALERT type 4 Improvement, methodology, query or suggestion
 3 ALERT type 5 Informative message, check

Datablock: 7

Bond precision: C-C = 0.0114 Å Wavelength=0.71073
 Cell: a=27.4177(12) b=8.2315(3) c=13.7691(7)
 alpha=90 beta=94.263(5) gamma=90
 Temperature: 293 K

	Calculated	Reported
Volume	3098.9(2)	3098.9(2)
Space group	C 2	C 2
Hall group	C 2y	C 2y
Moiety formula	C60 H42 Cd3 N12 O16, 4(H2 O)	?
Sum formula	C60 H50 Cd3 N12 O20	C60 H50 Cd3 N12 O20
Mr	1596.35	1596.35
Dx, g cm ⁻³	1.711	1.711
Z	2	2
Mu (mm ⁻¹)	1.107	1.107
F000	1596.0	1596.0
F000'	1591.88	
h, k, lmax	32, 9, 16	32, 9, 16
Nref	5443[2931]	5169
Tmin, Tmax	0.838, 0.895	0.838, 0.895
Tmin'	0.838	

Correction method= MULTI-SCAN

Data completeness= 1.76/0.95 Theta(max)= 25.000

R(reflections)= 0.0464(4455) wR2(reflections)= 0.1043(5169)

S = 1.044 Npar= 429

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	09	-	H9A	...	Please Check
PLAT420_ALERT_2_B D-H Without Acceptor	010	-	H10B	...	Please Check

● Alert level C

PLAT048_ALERT_1_C	MoietyFormula Not Given	Please Do !
PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	6.83
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.58
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O2 -- C1 ..	5.7 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Cd1 -- O2 ..	9.0 su
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	01 Check
PLAT241_ALERT_2_C	High Ueq as Compared to Neighbors for	02 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	Cd1 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	C1 Check
PLAT242_ALERT_2_C	Low Ueq as Compared to Neighbors for	C15 Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0114 Ang.
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .	31 Ang3
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #	1
C60 H42 Cd3 N12 O16		

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	9 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1
PLAT004_ALERT_5_G	Polymeric Structure Found with Dimension	3 Info
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6 Why ?
PLAT093_ALERT_1_G	No su's on H-positions, refinement reported as .	mixed
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.15 Ratio
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2
H2 O		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3
H2 O		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	16 Note

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

- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
13 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
4 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

checkCIF publication errors

● Alert level A

PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

Alert level G

PUBL017_ALERT_1_G The _publ_section_references section is missing or empty.

4 **ALERT level A** = Data missing that is essential or data in wrong format

1 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

```
# start Validation Reply Form
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PLAT415_2
;
PROBLEM: Short Inter D-H..H-X      H9      ..  H10A      ..      1.79 Ang.
RESPONSE: ...
;
_vrf_PLAT417_2
;
```

PROBLEM: Short Inter D-H...H-D H8A .. H11A .. 1.73 Ang.
RESPONSE: ...
;
end Validation Reply Form

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 18/09/2013; check.def file version of 12/09/2013

Datablock 1 - ellipsoid plot













