

checkCIF/PLATON report

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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 = 0.0025 A

Wavelength=0.71073

Cell: a=7.4145(11) b=7.6738(11) c=10.6697(15)
alpha=88.064(4) beta=82.611(4) gamma=74.497(4)
Temperature: 298 K

	Calculated	Reported
Volume	580.13(15)	580.13(14)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C18 H16 Cd N6 O8 S2	?
Sum formula	C18 H16 Cd N6 O8 S2	C18 H16 Cd N6 O8 S2
Mr	620.90	620.89
Dx, g cm-3	1.777	1.777
Z	1	1
Mu (mm-1)	1.179	1.179
F000	310.0	310.0
F000'	309.57	
h, k, lmax	9, 9, 13	9, 9, 13
Nref	2676	2614
Tmin, Tmax	0.797, 0.878	0.773, 0.881
Tmin'	0.762	

Correction method= # Reported T Limits: Tmin=0.773 Tmax=0.881
AbsCorr = MULTI-SCAN

Data completeness= 0.977

Theta(max)= 27.570

R(reflections)= 0.0205(2544)

wR2(reflections)= 0.0545(2614)

S = 1.123

Npar= 160

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 C

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full value Low .	0.977	Note
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● Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please	Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	2	Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.004	Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cd1 -- 04 ..	5.1	s.u.
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	5	Do !
	N1 -CD1 -N1 -C5 11.00 0.00 2.567 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	10	Do !
	N1 -CD1 -N1 -C1 8.00 0.00 2.567 1.555 1.555	1.555	
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note

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1 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
3 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

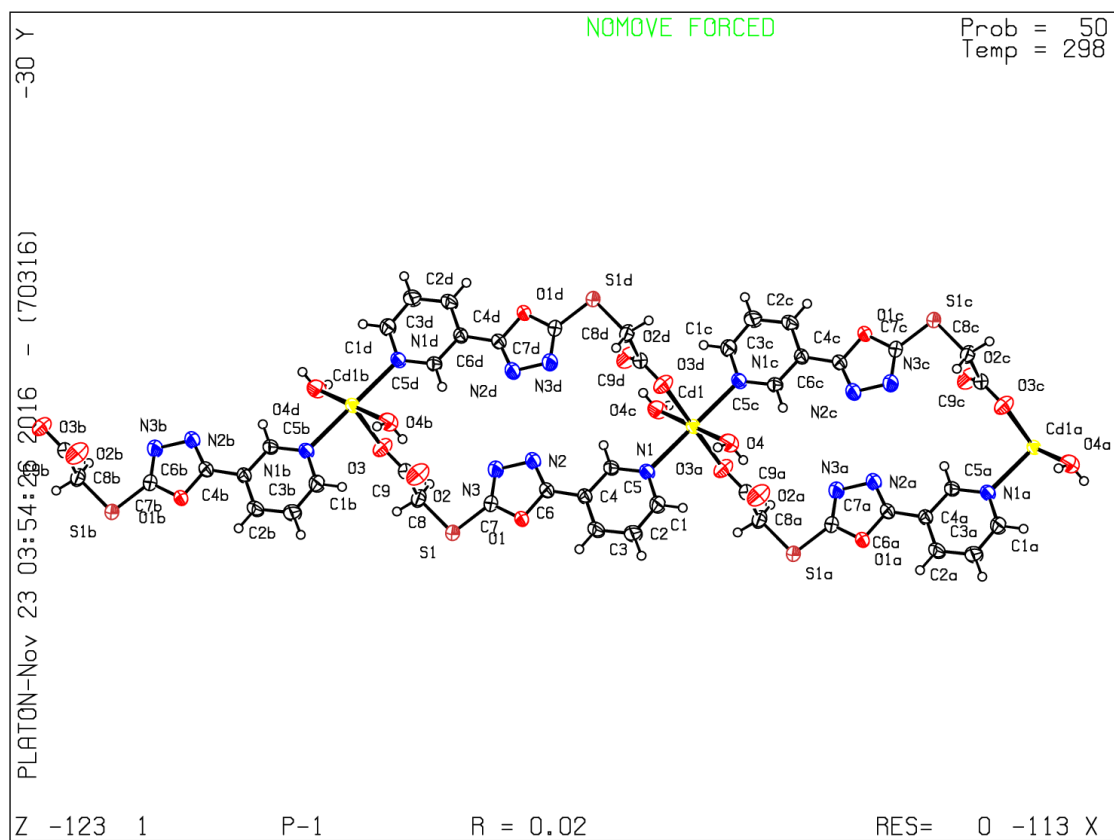
Publication of your CIF in IUCr journals

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.

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Datablock 1 - ellipsoid plot



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No syntax errors found.

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: 1

Bond precision: C-C = 0.0025 A

Wavelength=0.71073

Cell: a=7.3585(6) b=7.4216(7) c=10.7069(9)
alpha=88.979(3) beta=82.757(2) gamma=73.709(3)
Temperature: 298 K

	Calculated	Reported
Volume	556.67(8)	556.67(8)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C18 H16 N6 O8 S2 Zn	?
Sum formula	C18 H16 N6 O8 S2 Zn	C18 H16 N6 O8 S2 Zn
Mr	573.88	573.86
Dx, g cm-3	1.712	1.712
Z	1	1
Mu (mm-1)	1.351	1.351
F000	292.0	292.0
F000'	292.65	
h, k, lmax	9, 9, 13	9, 9, 13
Nref	2577	2531
Tmin, Tmax	0.850, 0.874	0.720, 0.877
Tmin'	0.704	

Correction method= # Reported T Limits: Tmin=0.720 Tmax=0.877
AbsCorr = MULTI-SCAN

Data completeness= 0.982

Theta(max)= 27.570

R(reflections)= 0.0245(2295)

wR2(reflections)= 0.0636(2531)

S = 1.080

Npar= 157

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 C

<u>PLAT165_ALERT_3_C</u>	Nr. of Status R Flagged Non-Hydrogen Atoms	1 Note
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Alert level G

<u>PLAT004_ALERT_5_G</u>	Polymeric Structure Found with Maximum Dimension	1 Info
<u>PLAT005_ALERT_5_G</u>	No Embedded Refinement Details found in the CIF	Please Do !
<u>PLAT007_ALERT_5_G</u>	Number of Unrefined Donor-H Atoms	2 Report
<u>PLAT093_ALERT_1_G</u>	No s.u.'s on H-positions, Refinement Reported as	mixed Check
<u>PLAT710_ALERT_4_G</u>	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	21 Do !
	N1 -ZN1 -N1 -C5 7.00 0.00 2.755 1.555 1.555 1.555	
<u>PLAT710_ALERT_4_G</u>	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	26 Do !
	N1 -ZN1 -N1 -C1 11.00 0.00 2.755 1.555 1.555 1.555	
<u>PLAT899_ALERT_4_G</u>	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

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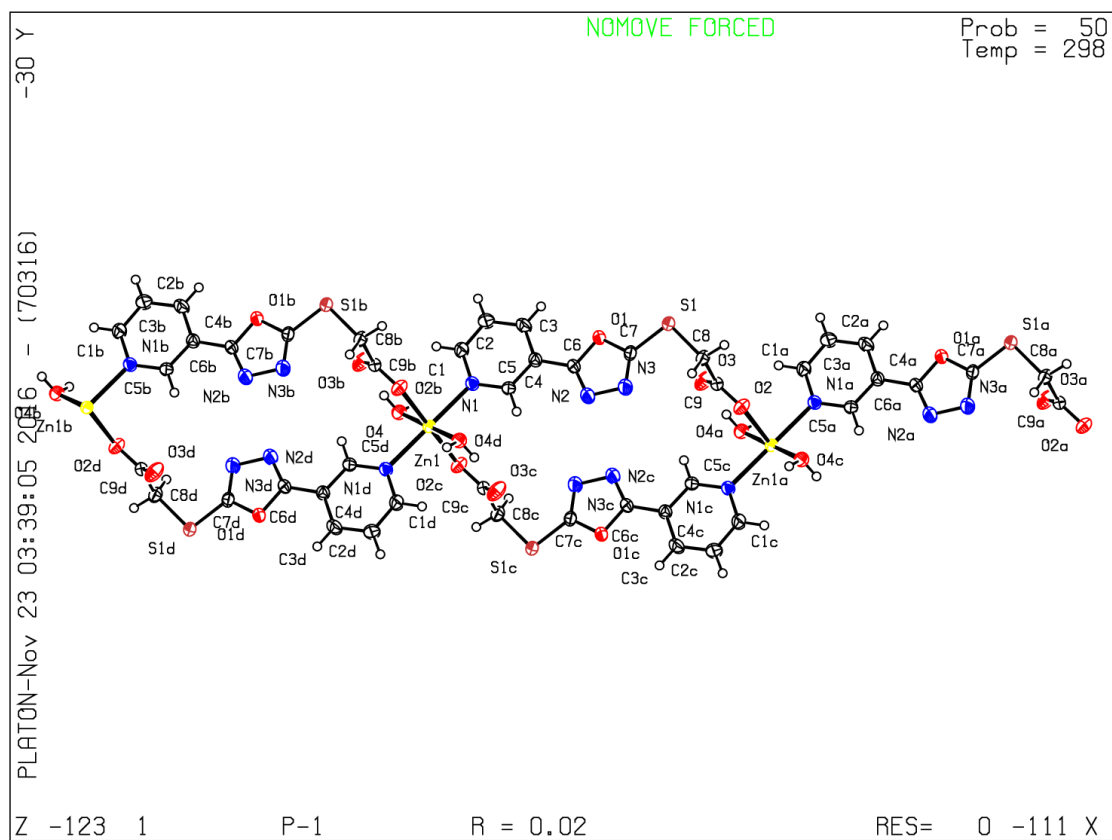
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[CIF dictionary](#)

[Interpreting this report](#)

Datablock: 2

Bond precision: C-C = 0.0019 A

Wavelength=0.71073

Cell: a=25.302(3)

b=10.6816(11)

c=7.1462(7)

alpha=90

beta=95.747(3)

gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	1921.7(4)	1921.7(3)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C18 H12 Mn N6 O6 S2	?
Sum formula	C18 H12 Mn N6 O6 S2	C18 H12 Mn N6 O6 S2
Mr	527.40	527.40
Dx, g cm-3	1.823	1.823
Z	4	4
Mu (mm-1)	0.960	0.960
F000	1068.0	1068.0
F000'	1070.75	
h, k, lmax	32, 13, 9	32, 13, 9
Nref	2224	2207
Tmin, Tmax	0.803, 0.866	0.809, 0.869
Tmin'	0.802	

Correction method= # Reported T Limits: Tmin=0.809 Tmax=0.869

AbsCorr = MULTI-SCAN

Data completeness= 0.992

Theta(max)= 27.550

R(reflections)= 0.0248(2080)

wR2(reflections)= 0.0679(2207)

S = 1.107

Npar= 150

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test-name_ALERT_alert-type_alert-level.

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● Alert level C

<u>PLAT250_ALERT_2_C</u>	Large U3/U1 Ratio for Average U(i,j) Tensor	2.7 Note
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● Alert level G

<u>PLAT004_ALERT_5_G</u>	Polymeric Structure Found with Maximum Dimension	3 Info
<u>PLAT005_ALERT_5_G</u>	No Embedded Refinement Details found in the CIF	Please Do !
<u>PLAT066_ALERT_1_G</u>	Predicted and Reported Tmin&Tmax Range Identical	? Check
<u>PLAT899_ALERT_4_G</u>	SHELXL97 is Deprecated and Succeeded by SHELXL	2014 Note

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