

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SH6

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: SH6

Bond precision:	O- C = 0.0050 A	Wavelength=1.54184
Cell:	a=16.5270 (5) alpha=90	b=6.0073 (2) beta=90
Temperature:	120 K	c=8.6821 (3) gamma=90
	Calculated	Reported
Volume	861.98 (5)	861.98 (5)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P -2xabc;-
Moiety formula	C8 H23 Cl2 Cu2 N4 O2, 2 (Cl)	C4 H12 Cl Cu N2 O, Cl
Sum formula	C8 H23 Cl4 Cu2 N4 O2	C4 H12 Cl2 Cu N2 O
Mr	476.20	238.60
Dx, g cm ⁻³	1.835	1.839
Z	2	4
Mu (mm ⁻¹)	8.802	8.802
F000	482.0	484.0
F000'	477.75	
h, k, lmax	19, 7, 10	19, 7, 10
Nref	856	855
Tmin, Tmax	0.115, 0.258	0.121, 0.427
Tmin'	0.021	

Correction method= # Reported T Limits: Tmin=0.121 Tmax=0.427
AbsCorr = ANALYTICAL

Data completeness= 0.999 Theta (max)= 67.250

R(reflections)= 0.0304 (794)	wR2(reflections)= 0.0907 (855)
S = 1.660	Npar= 78

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

PLAT110_ALERT_2_B ADDSYM Detects Potential Lattice Translation ... ? Check

Author Response: Hlaving the lattice parameter would introduce disorder of O1 and N2. Furthermore, although the reflections supporting the current a lattice parameter are less numerous than the rest, they are clearly observed.

PLAT112_ALERT_2_B ADDSYM Detects New (Pseudo) Symm. Elem a/2 100 %Fit

Author Response: Hlaving the lattice parameter would introduce disorder of O1 and N2. Furthermore, although the reflections supporting the current a lattice parameter are less numerous than the rest, they are clearly observed.

PLAT113_ALERT_2_B ADDSYM Suggests Possible Pseudo/New Space Group Pmmn Check
Note: (Pseudo) Lattice Translation Implemented

Author Response: Hlaving the lattice parameter would introduce disorder of O1 and N2. Furthermore, although the reflections supporting the current a lattice parameter are less numerous than the rest, they are clearly observed.

Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight	Differ by ..	1.00 Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT076_ALERT_1_C	Occupancy	0.500 Less Than 1.0 for Sp.pos	H1C2
PLAT127_ALERT_1_C	Implicit Hall Symbol	Inconsistent with Explicit	-P -2xa bc;-2yb
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		N2 Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N2 --H1N2	Please Check
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H1N2 ..CL1	2.92 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H1N2 ..CL2	2.88 Ang.
PLAT926_ALERT_1_C	Reported and Calculated	R1 Differ by	-0.0012 Check
PLAT927_ALERT_1_C	Reported and Calculated	wR2 Differ by	-0.0021 Check

Alert level G

PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula	Strings Differ	Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z	Differ by a Factor ...	0.50 Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cu1 --N1	5.4 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of C2	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1N1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1C1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2C1	Constrained at	0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H1C3	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2C3	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1C4	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2C4	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1C2	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2C2	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	40%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 1)	20.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 2)	0.50	Check
PLAT414_ALERT_2_G	Short Intra D-H..H-X	H1N2 ..H2C4	2.06	Ang.
		x,y,z =	1_555	Check
PLAT414_ALERT_2_G	Short Intra D-H..H-X	H1N2 ..H1C4	2.07	Ang.
		x,1/2-y,z =	7_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		11	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		32.20	Deg.
	C2 -N1 -C2	1_555 1_555 7_555	# 21	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		31.80	Deg.
	C3 -N1 -C3	1_555 1_555 7_555	# 30	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		31.10	Deg.
	C2 -C1 -C2	1_555 1_555 7_555	# 48	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		31.35	Deg.
	H1C1 -C1 -H2C1	1_555 1_555 7_555	# 59	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		31.35	Deg.
	H1C1 -C1 -H2C1	7_555 1_555 1_555	# 60	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		0.74	Deg.
	H1C2 -C2 -H1C2	1_555 1_555 7_555	# 75	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		2.89	Deg.
	H2C3 -C3 -H2C3	1_555 1_555 7_555	# 92	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		30.40	Deg.
	C3 -C4 -C3	1_555 1_555 7_555	# 99	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		31.31	Deg.
	H1C4 -C4 -H2C4	1_555 1_555 7_555	# 110	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		31.31	Deg.
	H1C4 -C4 -H2C4	7_555 1_555 1_555	# 111	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		4	Note
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		91%	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of		3.0	Sig(I)

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 3 **ALERT level B** = A potentially serious problem, consider carefully
 11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 35 **ALERT level G** = General information/check it is not something unexpected
- 10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 8 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
 26 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check
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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.

