

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelxl

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: shelxl

Bond precision: C-C = 0.0056 A Wavelength=0.71070

Cell: a=11.8583(2) b=14.6280(2) c=20.1371(3)
 alpha=90 beta=90 gamma=90
Temperature: 113 K

	Calculated	Reported
Volume	3493.05(9)	3493.05(9)
Space group	P 21 21 21	P212121
Hall group	P 2ac 2ab	?
Moiety formula	C30 H30 Cl4 Cu2 N4 O6	C30 H30 Cl4 Cu2 N4 O6
Sum formula	C30 H30 Cl4 Cu2 N4 O6	C30 H30 Cl4 Cu2 N4 O6
Mr	811.48	811.46
Dx,g cm-3	1.543	1.543
Z	4	4
Mu (mm-1)	1.570	1.570
F000	1648.0	1648.0
F000'	1653.43	
h,k,lmax	16,20,27	15,19,27
Nref	9501[5259]	7986
Tmin,Tmax	0.738,0.731	0.980,0.990
Tmin'	0.723	

Correction method= # Reported T Limits: Tmin=0.980 Tmax=0.990
AbsCorr = MULTI-SCAN

Data completeness= 1.52/0.84 Theta(max)= 29.240

R(reflections)= 0.0404(7201) wR2(reflections)= 0.1000(7986)

S = 1.064 Npar= 502

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

PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)	3	Report
PLAT220_ALERT_2_B	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	7.4	Ratio
PLAT391_ALERT_3_B	Deviating Methyl C27 H-C-H Bond Angle	96	Degree

Alert level C

DIFMX01_ALERT_2_C	The maximum difference density is > 0.1*ZMAX*0.75 _refine_diff_density_max given = 2.182 Test value = 2.175		
DIFMX02_ALERT_1_C	The maximum difference density is > 0.1*ZMAX*0.75 The relevant atom site should be identified.		
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ...	3.91	Report
PLAT222_ALERT_3_C	Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range	10.0	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	N1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C20	Check
PLAT245_ALERT_2_C	U(iso) H28 Smaller than U(eq) C25 by ...	0.017	AngSq
PLAT245_ALERT_2_C	U(iso) H38A Smaller than U(eq) C29 by ...	0.019	AngSq
PLAT245_ALERT_2_C	U(iso) H38B Smaller than U(eq) C29 by ...	0.014	AngSq
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C30 - H31B ..	1.12	Ang.
PLAT390_ALERT_3_C	Deviating Methyl C29 X-C-H Bond Angle	103	Degree
PLAT390_ALERT_3_C	Deviating Methyl C30 X-C-H Bond Angle	102	Degree
PLAT391_ALERT_3_C	Deviating Methyl C27 H-C-H Bond Angle	118	Degree
PLAT391_ALERT_3_C	Deviating Methyl C29 H-C-H Bond Angle	117	Degree
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min)	6	Note
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	79	%
PLAT971_ALERT_2_C	Check Calcd Residual Density 0.10A From C19B	2.36	eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on H5A	-0.49	eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on H5B	-0.44	eA-3

Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF	Please	Do !
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	22	Note
PLAT301_ALERT_3_G	Main Residue Disorder	7	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	2	Note
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF # C24B -N1 -C24A 1.555 1.555 1.555	22.10	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF # C23A -N1 -C23B 1.555 1.555 1.555	35.80	Deg.
PLAT791_ALERT_4_G	The Model has Chirality at C8 (Chiral SPGR)	S	Verify
PLAT791_ALERT_4_G	The Model has Chirality at C17 (Chiral SPGR)	S	Verify
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	592	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density	2	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
19 **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

1 **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
11 **ALERT type 3** Indicator that the structure quality may be low
8 **ALERT type 4** Improvement, methodology, query or suggestion
1 **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.

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