

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ras1306_squeeze

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: ras1306_squeeze

Bond precision:	C-C = 0.0060 Å	Wavelength=0.71073	
Cell:	a=13.3604(3)	b=8.8530(1)	c=16.6709(4)
	alpha=90	beta=95.0682(9)	gamma=90
Temperature:	200 K		
	Calculated	Reported	
Volume	1964.12(7)	1964.12(7)	
Space group	P 2/n	P 1 2/n 1	
Hall group	-P 2yac	-P 2yac	
Moiety formula	C20 H32 Cl6 Cu4 N8 O	C20 H32 Cl6 Cu4 N8 O	
Sum formula	C20 H32 Cl6 Cu4 N8 O	C20 H32 Cl6 Cu4 N8 O	
Mr	867.44	867.43	
Dx, g cm-3	1.467	1.467	
Z	2	2	
Mu (mm-1)	2.569	2.569	
F000	868.0	868.0	
F000'	872.45		
h, k, lmax	17, 11, 21	17, 11, 21	
Nref	4531	4523	
Tmin, Tmax	0.742, 0.835	0.503, 0.848	
Tmin'	0.320		

Correction method= # Reported T Limits: Tmin=0.503 Tmax=0.848
AbsCorr = INTEGRATION

Data completeness= 0.998 Theta(max)= 27.505

R(reflections)= 0.0426(4041) wR2(reflections)= 0.1077(4519)

S = 1.001 Npar= 182

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

PLAT902_ALERT_1_A No (Interpretable) Reflections found in FCF Please Check

Alert level C

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Cl1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cu2 Check

Alert level G

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
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.02 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 -- Cl1 .. 6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 -- Cl2_a .. 17.4 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of *Cl4 is Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder Percentage = 3 Note
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl3 .. Cl4 .. 3.28 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl3 .. Cl4 .. 3.28 Ang.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in Structure ... 227 A**3
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.16 Ratio
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed ! Info

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **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
7 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
4 ALERT type 4 Improvement, methodology, query or suggestion
2 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*, 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.

