

checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: kcd1055

Bond precision:	C-C = 0.0073 A	Wavelength=0.71073	
Cell:	a=18.854(9)	b=16.428(8)	c=15.648(8)
	alpha=90	beta=96.55(4)	gamma=90
Temperature:	123 K		
	Calculated	Reported	
Volume	4815(4)	4815(4)	
Space group	P 21/c	P 21/c	
Hall group	2ybc	2ybc	
Moiety formula	C42 H32 Cr2 N10 O S2, 2(Cl O4), 2(H2 O)	C42 H36 Cl2 Cr2 N10 O11 S2	
Sum formula	C42 H36 Cl2 Cr2 N10 O11 S2	C42 H36 Cl2 Cr2 N10 O11 S2	
Mr	1095.85	1095.92	
Dx,g cm-3	1.512	1.512	
Z	4	4	
Mu (mm-1)	0.718	0.720	
F000	2240.0	2384.0	
F000'	2245.60		
h,k,lmax	22,19,18	21,19,18	
Nref	8783	8254	
Tmin,Tmax	0.784,0.967	0.743,0.965	
Tmin'	0.750		

Correction method= INTEGRATION

Data completeness= 0.940 Theta(max)= 25.310

R(reflections)= 0.0583(6348) wR2(reflections)= 0.1649(8254)


S = 1.046 Npar= 634

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


RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.281

 **Alert level B**

PLAT029_ALERT_3_B	_diffn_measured_fraction_theta_full	Low	0.940
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H10B	.. H11A ..	2.09 Ang.

 **Alert level C**

PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	?
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0073 Ang

 **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	?
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	?
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	23.73
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	6

- | | |
|---|---|
| 1 | ALERT level A = Most likely a serious problem - resolve or explain |
| 2 | ALERT level B = A potentially serious problem, consider carefully |
| 2 | ALERT level C = Check. Ensure it is not caused by an omission or oversight |
| 5 | ALERT level G = General information/check it is not something unexpected |
| | |
| 2 | ALERT type 1 CIF construction/syntax error, inconsistent or missing data |
| 3 | 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 |
| 0 | 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*, 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.

Datablock kcd1055 - ellipsoid plot

