

checkCIF/PLATON report

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

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: pnaa

Bond precision:	C-C = 0.0168 A	Wavelength=0.71073	
Cell:	a=14.5317(4)	b=26.9817(7)	c=14.8316(4)
	alpha=90	beta=90	gamma=90
Temperature:	298 K		
	Calculated	Reported	
Volume	5815.3(3)	5815.3(3)	
Space group	P n n a	Pnaa	
Hall group	-P 2a 2bc	?	
Moiety formula	C31 H23 Cl2 Co N4 O2	?	
Sum formula	C31 H23 Cl2 Co N4 O2	C31 H23 Cl2 Co N4 O2	
Mr	613.36	613.36	
Dx,g cm-3	1.401	1.401	
Z	8	8	
Mu (mm-1)	0.809	0.809	
F000	2512.0	2512.0	
F000'	2517.91		
h,k,lmax	17,33,18	17,33,18	
Nref	5717	5713	
Tmin,Tmax	0.824,0.893	0.690,0.746	
Tmin'	0.817		

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.000

R(reflections)= 0.0987(4460) wR2(reflections)= 0.2432(5713)

S = 1.162 Npar= 371

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**

PLAT215_ALERT_3_B	Disordered C16A	has ADP max/min Ratio	4.2	
PLAT220_ALERT_2_B	Large Non-Solvent	C	Ueq(max)/Ueq(min)	...	5.4 Ratio
PLAT234_ALERT_4_B	Large Hirshfeld Difference	C15	-- C16	..	0.26 Ang.
PLAT341_ALERT_3_B	Low Bond Precision on	C-C Bonds		0.0168 Ang.

● **Alert level C**

PLAT213_ALERT_2_C	Atom C15A	has ADP max/min Ratio	3.1	prola
PLAT222_ALERT_3_C	Large Non-Solvent	H	Uiso(max)/Uiso(min)	..	5.7 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C7A	-- C12A	..	0.16 Ang.
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for		C15	
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for		C14A	
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j)	Tensor	2.6	
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond	C15A	- C15A_b	...	1.53 Ang.

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			2	
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF			?	Do !
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.			51.62	
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C15A	-- C16A	..	5.2 su
PLAT301_ALERT_3_G	Note: Main Residue Disorder		3	%
PLAT335_ALERT_2_G	Check Large C6 Ring	C-C Range	C13A -C13A_b		0.19 Ang.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints		1	

0 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
2 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.

