

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait ..

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) IG3

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.

Please wait while processing

[report](#)

[Structure factor report](#)

[CIF dictionary](#)

[Interpreting this](#)

Datablock: IG3

Bond precision:	C-C = 0.0055 Å	Wavelength=0.71073
Cell:	a=22.0311 (7) b=12.2362 (4) c=8.1475 (3)	
	alpha=90 beta=90 gamma=90	
Temperature:	100 K	
	Calculated	Reported
Volume	2196.38 (13)	2196.38 (13)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C8 H10 Cl2 N6 O4 Pt, 2 (C3 H6 O)	C8 H10 Cl2 N6 O4 Pt, 2 (C3 H6 O)
Sum formula	C14 H22 Cl2 N6 O6 Pt	C14 H22 Cl2 N6 O6 Pt
Mr	636.36	636.36
Dx, g cm ⁻³	1.924	1.924
Z	4	4
Mu (mm ⁻¹)	6.673	6.673
F000	1232.0	1232.0
F000'	1227.09	
h, k, lmax	29, 16, 11	29, 16, 10
Nref	2881	2571
Tmin, Tmax	0.453, 0.819	0.789, 0.897
Tmin'	0.318	
Correction method=	# Reported T Limits: Tmin=0.789	
Tmax=0.897 AbsCorr =	ANALYTICAL	
Data completeness=	0.892	Theta(max)= 28.891
R(reflections)=	0.0263 (1810)	wR2(reflections)= 0.0542 (2571)
S =	1.033	Npar= 136

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 C

[PLAT906 ALERT 3 C](#) Large K Value in the Analysis of Variance
6.170 Check
[PLAT906 ALERT 3 C](#) Large K Value in the Analysis of Variance
2.170 Check

● Alert level G

[PLAT432 ALERT 2 G](#) Short Inter X...Y Contact 0006 ..C00D
2.98 Ang.
$$x,1-y,1/2+z = 7_566$$

Check
[PLAT720 ALERT 4 G](#) Number of Unusual/Non-Standard Labels
27 Note
[PLAT794 ALERT 5 G](#) Tentative Bond Valency for Pt01 (II) .
2.22 Info
[PLAT883 ALERT 1 G](#) No Info/Value for _atom_sites_solution_primary .
Please Do !
[PLAT910 ALERT 3 G](#) Missing # of FCF Reflection(s) Below Theta(Min).
3 Note
[PLAT912 ALERT 4 G](#) Missing # of FCF Reflections Above STh/L= 0.600
305 Note
[PLAT941 ALERT 3 G](#) Average HKL Measurement Multiplicity
2.8 Low
[PLAT978 ALERT 2 G](#) Number C-C Bonds with Positive Residual Density.
1 Info

0 **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

8 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

2 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

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

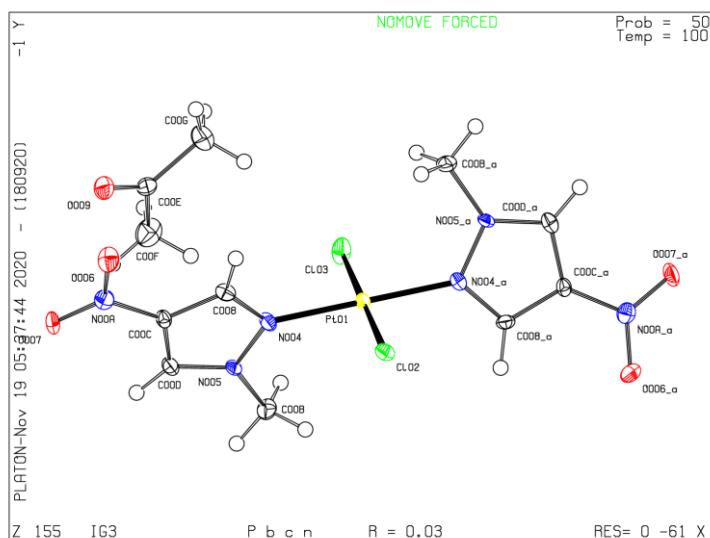
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* 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.

PLATON version of 18/09/2020; check.def file version of 20/08/2020

Datablock IG3 - ellipsoid plot



Download CIF editor (publCIF) from the IUCr

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[Test a new CIF entry](#)