

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: 1

Bond precision:	C-C = 0.0271 A	Wavelength=0.71073
Cell:	a=9.8798 (13)	b=14.6422 (19) c=18.604 (2)
	alpha=107.068 (3)	beta=97.771 (3) gamma=102.798 (3)
Temperature:	193 K	
	Calculated	Reported
Volume	2450.3 (5)	2450.2 (6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C54 H36 Cl2 N4 O4 P2 Pt2 [+ solvent]	C54 H36 Cl2 N4 O4 P2 Pt2
Sum formula	C54 H36 Cl2 N4 O4 P2 Pt2 [+ solvent]	C54 H36 Cl2 N4 O4 P2 Pt2
Mr	1327.87	1327.89
Dx, g cm ⁻³	1.800	1.800
Z	2	2
Mu (mm ⁻¹)	5.928	5.928
F000	1280.0	1280.0
F000'	1274.84	
h, k, lmax	11, 17, 22	11, 17, 22
Nref	8636	8627
Tmin, Tmax	0.454, 0.491	
Tmin'	0.419	

Correction method= Not given

Data completeness= 0.999 Theta(max)= 24.999

R(reflections)= 0.0834 (5292)

wR2(reflections)=
0.2588 (8627)

S = 1.024

Npar= 613

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

PLAT234_ALERT_4_B	Large Hirshfeld Difference C46	--C47	.	0.26 Ang.
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds			0.02714 Ang.
PLAT990_ALERT_1_B	Deprecated .res/.hkl Input Style SQUEEZE Job ...			! Note

Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given		Please Do !
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)			0.26 Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density			3.83 Report
PLAT213_ALERT_2_C	Atom C34	has ADP max/min Ratio		3.2 prolat
PLAT234_ALERT_4_C	Large Hirshfeld Difference C1	--C2	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C5	--C6	.	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C9	--C10	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C14	--C15	.	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C24	--C25	.	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C53	--C54	.	0.19 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			C34 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			C36 Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)			2.4 Note
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4			Please Check

Alert level G

PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H Atoms			62 Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large			0.16 Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)			0.003 Degree
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records			1 Report
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C23	-C27	.	1.46 Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C13	-C18		0.19 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact O3	..C39	.	2.97 Ang.
		x,l+y,z =		1_565 Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure			263 A**3
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			396 Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed			! Info
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			2 Note
	2 -3 5, -3 13 3,			
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			3.5 Low
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..			50.0 Degree

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

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

11 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
11 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 22/08/2024; check.def file version of 21/08/2024

Datablock 1 - ellipsoid plot

