

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: shelx

Bond precision: C-C = 0.0212 A Wavelength=0.71073

Cell: a=20.3117(19) b=21.479(2) c=23.204(2)
 alpha=109.568(3) beta=105.798(3) gamma=103.892(3)

Temperature: 110 K

	Calculated	Reported
Volume	8543.7(14)	8543.9(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C88 H92 Au2 N8 P4, C H2 Cl2, 2(Cl) [+ solvent]	C88 H92 Au2 N8 P4, C H2 Cl2, 2(Cl)
Sum formula	C89 H94 Au2 Cl4 N8 P4 [+ solvent]	C89 H94 Au2 Cl4 N8 P4
Mr	1935.35	1935.33
Dx, g cm ⁻³	1.505	1.505
Z	4	4
Mu (mm ⁻¹)	3.679	3.679
F000	3880.0	3880.0
F000'	3869.18	
h, k, lmax	25, 26, 29	25, 26, 29
Nref	35465	35148
Tmin, Tmax	0.699, 0.929	0.579, 0.745
Tmin'	0.685	

Correction method= # Reported T Limits: Tmin=0.579 Tmax=0.745

AbsCorr = MULTI-SCAN

Data completeness= 0.991

Theta(max)= 26.513

R(reflections)= 0.0677(23952)

wR2(reflections)=
0.1766(35148)

S = 1.065

Npar= 1829

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

PLAT213_ALERT_2_B	Atom C12C	has ADP max/min Ratio	4.5	prolat
PLAT234_ALERT_4_B	Large Hirshfeld Difference	C27D	--C28D	.	0.28 Ang.
PLAT342_ALERT_3_B	Low Bond Precision on	C-C Bonds	0.02123	Ang.
PLAT410_ALERT_2_B	Short Intra H...H Contact	H44G	..H50D	.	1.88 Ang.
		x, y, z =		1_555	Check

● Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without a literature citation. This should be contained in the _exptl_absorpt_process_details field.

Absorption correction given as multi-scan

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.123

PLAT213_ALERT_2_C	Atom N46F	has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C	Atom C45F	has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C	Atom C47F	has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C	Atom C48F	has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C	Atom C49F	has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C	Atom C50F	has ADP max/min Ratio	3.9	prolat
PLAT213_ALERT_2_C	Atom C28C	has ADP max/min Ratio	3.5	prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1	C Ueq(max)/Ueq(min) Range	4.2	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 1	N Ueq(max)/Ueq(min) Range	4.4	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 2	C Ueq(max)/Ueq(min) Range	4.8	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 2	N Ueq(max)/Ueq(min) Range	3.3	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H Uiso(max)/Uiso(min) Range	4.3	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 2	H Uiso(max)/Uiso(min) Range	4.9	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	N1	--C8	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	N25B	--C24B	.	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C44	--C45	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	N25D	--C24D	.	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C13D	--C14D	.	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C39C	--C40C	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C43D	--C44D	.	0.18 Ang.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N25B	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C23B	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C28B	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C31B	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N25D	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C11C	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C12C	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C14D	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C26C	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C28D	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C44D	Check

PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C24B	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C26B	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C10C	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C14C	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C24C	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C29D	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of		C100	Check
PLAT260_ALERT_2_C	Large	Average	Ueq of Residue Including	C111	0.109	Check
PLAT331_ALERT_2_C	Small	Aver	Phenyl C-C Dist	C10C --C15C .	1.36	Ang.
PLAT411_ALERT_2_C	Short	Inter	H...H Contact	H11C ..H36B .	2.01	Ang.
				x,y,z =	1_555	Check

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				7	Note
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12				0.123	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large				119.24	Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)				0.003	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records				8	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records				4	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records				3	Report
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)			16%	Note
PLAT410_ALERT_2_G	Short Intra H...H Contact	H8A ..H44A .			2.01	Ang.
			x,y,z =		1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact	H8B1 ..H44C .			2.07	Ang.
			x,y,z =		1_555	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact	H14D ..H50E .			2.12	Ang.
			2-x,1-y,1-z =		2_766	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact	H40D ..H47E .			2.07	Ang.
			1-x,1-y,1-z =		2_666	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C114 ..C48B .			3.24	Ang.
			1-x,1-y,1-z =		2_666	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure				171	A**3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels				24	Note
PLAT722_ALERT_1_G	Angle Calc 122.00, Rep 123.40 Dev...				1.40	Degree
	C50E -C49E -H49E	1_555 1_555 1_555	#	647		Check
PLAT793_ALERT_4_G	Model has Chirality at C9C	(Centro SPGR)				R Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				13	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed				!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .					Please Do !
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File				62	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged					Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..				60.0	Degree

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

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
42 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
16 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT213_shelx
;
PROBLEM: Atom C12C          has ADP max/min Ratio .....      4.5 prolat
RESPONSE: ...
;
_vrf_PLAT234_shelx
;
PROBLEM: Large Hirshfeld Difference C27D    --C28D      .      0.28 Ang.
RESPONSE: ...
;
_vrf_PLAT342_shelx
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.02123 Ang.
RESPONSE: ...
;
_vrf_PLAT410_shelx
;
PROBLEM: Short Intra H...H Contact  H44G    ..H50D      .      1.88 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

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 18/05/2022; check.def file version of 17/05/2022

