

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

Bond precision: C-C = 0.0094 Å Wavelength=0.71073

Cell: a=12.0302(4) b=21.8633(7) c=28.1457(10)
 alpha=90 beta=90 gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	7402.9(4)	7402.9(4)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C55 H92 Au Cl N2 O28, C H Cl3	C55 H92 Au Cl N2 O28, C H Cl3
Sum formula	C56 H93 Au Cl4 N2 O28	C56 H93 Au Cl4 N2 O28
Mr	1581.10	1581.08
Dx, g cm ⁻³	1.419	1.419
Z	4	4
Mu (mm ⁻¹)	2.208	2.208
F000	3256.0	3256.0
F000'	3252.06	
h,k,lmax	16,30,38	16,30,38
Nref	20026[10889]	19999
Tmin,Tmax	0.735,0.820	0.581,0.746
Tmin'	0.695	

Correction method= # Reported T Limits: Tmin=0.581 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.84/1.00 Theta(max)= 29.186

R(reflections)= 0.0440(17821) wR2(reflections)= 0.1159(19999)

S = 1.076 Npar= 891

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

PLAT213_ALERT_2_C	Atom C9D	has ADP max/min Ratio	3.4	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1	C	Ueq(max) / Ueq(min) Range	5.4	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 1	O	Ueq(max) / Ueq(min) Range	3.8	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1	H	Uiso(max)/Uiso(min) Range	6.4	Ratio
PLAT242_ALERT_2_C	Low	MainMol	Ueq as Compared to Neighbors of	06E	Check
PLAT242_ALERT_2_C	Low	MainMol	Ueq as Compared to Neighbors of	C6B	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		Cl2	0.133	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		Cl5	0.137	Check
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.00935	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact	H6AA	..H5F	1.97	Ang.
			x,y,z =	1_555	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=		0.600	14	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.78A	From Aul	2.25	eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.			0	Info

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			11	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...			11	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large		7.95	Why ?
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records			3	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records			4	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records			1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records			2	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C9A2	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9A	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9AA	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9AB	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9AC	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9AD	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9AE	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9AF	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl2	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl3	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl4	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl5	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl6	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl7	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5	Constrained at		0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)		2%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)			100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)			100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 2)		2.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 3)		2.50	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3D			109.6	Degree
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H3A	..H9AC	2.11	Ang.
			x,y,z =	1_555	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H3D	..H9DC	1.87	Ang.
			x,y,z =	1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H1D	..H9AB	2.11	Ang.
			1-x,1/2+y,3/2-z =	3_656	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H7BA	..H9DD	2.01	Ang.

	1-x,-1/2+y,3/2-z =	3_646 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C12 ..C9A2		2.95 Ang.
	1-x,1/2+y,3/2-z =	3_656 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels		68 Note
PLAT722_ALERT_1_G Angle Calc 108.00, Rep 109.50 Dev...		1.50 Degree
H9DB -C9D -H9DC 1.555 1.555 1.555	# 240	Check
PLAT791_ALERT_4_G Model has Chirality at C1A	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C1B	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C1C	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C1D	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C1E	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C1F	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C2A	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C2B	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C2C	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C2D	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C2E	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C2F	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C3A	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C3B	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C3C	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C3D	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C3E	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C3F	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C4A	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C4B	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C4C	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C4D	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C4E	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C4F	(Chiral SPGR)	S Verify
PLAT791_ALERT_4_G Model has Chirality at C5A	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C5B	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C5C	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C5D	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C5E	(Chiral SPGR)	R Verify
PLAT791_ALERT_4_G Model has Chirality at C5F	(Chiral SPGR)	R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints		25 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).		2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		4 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF		1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...		19 Note
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by		2 Check

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 20 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
 58 ALERT type 4 Improvement, methodology, query or suggestion
 1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

PUBL004_ALERT_1_A The contact author's name and address are missing,
_publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A _publ_contact_author_email, _publ_contact_author_fax and
_publ_contact_author_phone are all missing.
At least one of these should be present.
PUBL006_ALERT_1_A _publ_requested_journal is missing
e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A _publ_section_abstract is missing.
Abstract of paper in English.

7 **ALERT level A** = Data missing that is essential or data in wrong format

0 **ALERT level G** = General alerts. Data that may be required is missing

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

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_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
```

```

;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form

```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

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