

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: nz1366_sqd

Bond precision: C-C = 0.0130 A

Wavelength=0.71073

Cell: a=15.2538(4) b=17.7777(7) c=25.8862(9)
 alpha=89.730(3) beta=72.967(3) gamma=82.322(3)
Temperature: 150 K

	Calculated	Reported
Volume	6647.3(4)	6647.3(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C125 H114 Cu3 N4 O6 P6 Re2), 2(F6 P), 4.5(C H2 Cl2)	?
Sum formula	C254.50 H237 Cl9 Cu6 F12 N8 O12 P14 Re4	C127.25 H118.50 Cl4.50 Cu3 F6 N4 O6 P7 Re2
Mr	5706.31	2853.09
Dx,g cm-3	1.426	1.425
Z	1	2
Mu (mm-1)	2.521	2.521
F000	2861.0	2861.0
F000'	2862.55	
h,k,lmax	20,23,34	20,23,33
Nref	32533	28214
Tmin,Tmax	0.682,0.838	0.703,1.000
Tmin'	0.410	

Correction method= # Reported T Limits: Tmin=0.703 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.867

Theta(max)= 28.137

R(reflections)= 0.0678(16798)

wR2(reflections)= 0.1856(28214)

S = 1.067

Npar= 1460

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**

PLAT029_ALERT_3_B	_diffn_measured_fraction_theta_full	Low	0.948	Note
PLAT220_ALERT_2_B	Large Non-Solvent	C	Ueq(max)/Ueq(min) Range	7.3	Ratio
PLAT222_ALERT_3_B	Large Non-Solvent	H	Uiso(max)/Uiso(min) ...	7.4	Ratio
PLAT242_ALERT_2_B	Low		Ueq as Compared to Neighbors for	C47	Check
PLAT242_ALERT_2_B	Low		Ueq as Compared to Neighbors for	C57	Check

● **Alert level C**

PLAT213_ALERT_2_C	Atom C18		has ADP max/min Ratio	3.5	prolat
PLAT213_ALERT_2_C	Atom C50		has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C60		has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C102		has ADP max/min Ratio	3.2	prolat
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Re2	-- C61 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O62	-- C61 ..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O66	-- C65 ..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C47	-- C49 ..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C57	-- C58 ..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C88	-- C93 ..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C100	-- C101 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C109	-- C110 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C121	-- C122 ..	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C127	-- C128 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C134	-- C135 ..	0.16	Ang.
PLAT241_ALERT_2_C	High		Ueq as Compared to Neighbors for	C74	Check
PLAT241_ALERT_2_C	High		Ueq as Compared to Neighbors for	C86	Check
PLAT241_ALERT_2_C	High		Ueq as Compared to Neighbors for	C102	Check
PLAT241_ALERT_2_C	High		Ueq as Compared to Neighbors for	C128	Check
PLAT241_ALERT_2_C	High		Ueq as Compared to Neighbors for	C131	Check
PLAT241_ALERT_2_C	High		Ueq as Compared to Neighbors for	C132	Check
PLAT241_ALERT_2_C	High		Ueq as Compared to Neighbors for	C140	Check
PLAT242_ALERT_2_C	Low		Ueq as Compared to Neighbors for	C17	Check
PLAT242_ALERT_2_C	Low		Ueq as Compared to Neighbors for	C70	Check
PLAT242_ALERT_2_C	Low		Ueq as Compared to Neighbors for	C100	Check
PLAT242_ALERT_2_C	Low		Ueq as Compared to Neighbors for	C127	Check
PLAT242_ALERT_2_C	Low		Ueq as Compared to Neighbors for	C130	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	C160	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.6	Note
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds			0.0130	Ang.
PLAT373_ALERT_2_C	Long C(sp)-C(sp) Bond	C2 - C3	...	1.38	Ang.
PLAT373_ALERT_2_C	Long C(sp)-C(sp) Bond	C6 - C7	...	1.38	Ang.
PLAT411_ALERT_2_C	Short Inter H...H Contact	H103 .. H121	..	2.14	Ang.

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			6	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...			3	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by			0.50	Ratio
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal			0.00300	Degree
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records			1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Re2	-- C65	..	6.2	su
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of			P150	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C116	is Constrained at		0.750	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C117	is Constrained at		0.750	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C161	is Constrained at		0.750	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of >H16C	is Constrained at	0.750	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >H16D	is Constrained at	0.750	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *Cl18	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *Cl19	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *Cl62	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H16E	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *H16F	is Constrained at	0.500	Check
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage =	27	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (3.75)	in Resd. #	4	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (2.50)	in Resd. #	5	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C4		Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C5		Check
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure			! Info
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	F6 P			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		3	Note
	C H2 C12			
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		21	Note
PLAT869_ALERT_4_G	ALERTS Related to the use of SQUEEZE Suppressed			! Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
28 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
31 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

PLATON version of 21/06/2015; check.def file version of 21/06/2015

